

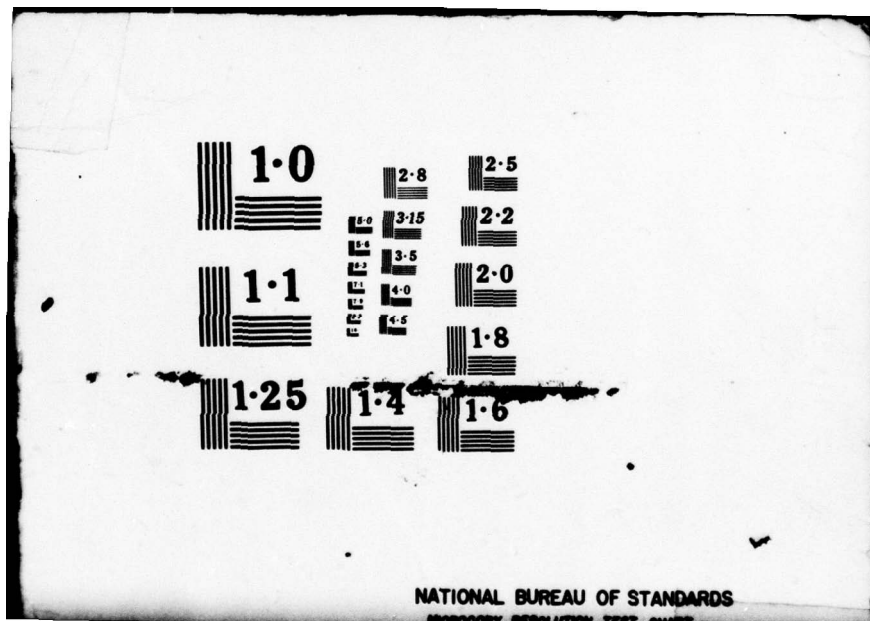
AD-A066 155

NORTHROP RESEARCH AND TECHNOLOGY CENTER PALOS VERDES --ETC F/G 20/5  
THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSES--ETC(U)  
JAN 79 W B LACINA  
N00014-78-C-0499  
NL

UNCLASSIFIED

1 OF 3  
ADA  
066155







**LEVEL III**

12  
B.S.

NRTC-79-7R

THEORETICAL MODELING OF MOLECULAR AND ELECTRON  
KINETIC PROCESSES

Volume I

Theoretical Formulation of Analysis and  
Description of Computer Programs

January, 1979

William B. Lacina

DDC  
REF ID: A66155  
MAR 21 1979  
C

DDC FILE COPY

This document has been approved  
for public release and sale; its  
distribution is unlimited.

Sponsored by

OFFICE OF NAVAL RESEARCH  
Department of the Navy

Contract No. N00014-78-C-0499

**NORTHROP**

Research and Technology Center

79 03 21 016

6

THEORETICAL MODELING OF MOLECULAR AND ELECTRON  
KINETIC PROCESSES.

Volume I.

Theoretical Formulation of Analysis and  
Description of Computer Program.

11

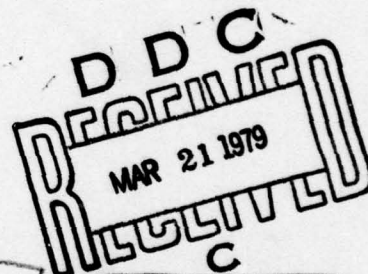
January, 1979

14

NRTZ-79-7R-VOL-1

10

William B. Lacina



9

Final technical rept. 12 Jun 78 - 15 Jan 79

12

248 p.

NORTHROP RESEARCH AND TECHNOLOGY CENTER  
One Research Park  
Palos Verdes Peninsula, California 90274  
Telephone: (213) 377-4811

This document has been approved  
for public release and sale; its  
distribution is unlimited.

Sponsored by

OFFICE OF NAVAL RESEARCH  
Department of the Navy

Contract No. N00014-78-C-0499

15

407 696 78 03 21 016.

slf



REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER NRTC-79-7R	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSES Vol. I: Theoretical Formulation of Analysis and Description of Computer Programs		5. TYPE OF REPORT & PERIOD COVERED Final Technical Report 12 June 1978 to 15 Jan. 1979
7. AUTHOR(s) William B. Lacina AD-A066156		6. PERFORMING ORG. REPORT NUMBER NRTC-79-7R
8. PERFORMING ORGANIZATION NAME AND ADDRESS NORTHROP Research & Technology Center One Research Park Palos Verdes Peninsula, Calif. 90274		9. CONTRACT OR GRANT NUMBER(s) N00014-78-C-0499 <i>new</i>
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research, Dept. of the Navy 800 N. Quincy Street Arlington, Virginia 22217		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Attn.: 613C:MAK
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) Office of Naval Research, Pasadena, Calif.		12. REPORT DATE January, 1979
		13. NUMBER OF PAGES 234
		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Unlimited.		
<div style="border: 1px solid black; padding: 5px; text-align: center;"> <b>DISTRIBUTION STATEMENT A</b>          Approved for public release;          Distribution Unlimited       </div>		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Molecular kinetics, electron kinetics, Boltzmann equation, laser kinetics, transient analysis, electrically excited laser, KrF laser, rare gas halides, kinetic modeling, superelastic collisions, electron-electron collisions		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report describes and documents a comprehensive and reasonably general computer analysis applicable to a broad class of transient, electrically excited laser systems. The theoretical model is formulated, for a spatially homogeneous medium, in terms of the coupled set of equations which describe the molecular kinetics, electron kinetics, external discharge circuit, and optical radiative extraction. One of the unique features of the present code is that the molecular kinetic subroutines for an arbitrary reaction scheme are synthesized auto-		

matically by translation of an input queue of symbolically expressed reactions into computer-coded FORTRAN equations, which are automatically coupled to a Boltzmann analysis of electron kinetics.)

The molecular kinetics reaction scheme is translated into subroutines which produce the instantaneous rates  $n_i$  and the Jacobian  $\delta \dot{n}_i / \delta n_j$  (for the population densities and electrical circuit parameters) so that a multistep Gear technique can be implemented for integration of the ("stiff") system of coupled equations. The radiation fields for laser extraction are formulated in terms of the intracavity photon density, with a source term from spontaneous noise and amplification (and absorption) by the excited medium. This approach allows radiation, electrons, and all of the other molecular "species" to be treated on a parallel basis.

→ The electron kinetics analysis consists of numerical solution of the Boltzmann equation for the electron energy distribution. The technique for solution permits inclusion of inelastic binary electron-molecule collisions, superelastic collisions, electron-electron collisions, momentum transfer (with recoil), a source term  $S_0 \delta(u) + S_1 s(u)$  for external creation of electrons (at zero energy and over a distribution of energies) by sources of ionization, and retention of the term proportional to  $dn_e/dt$  for situations involving a net change in the electron density. From the electron <sup>sub e</sup> energy distribution, all of the plasma parameters, electron excitation rates, and power partitioning can be obtained. ←

The general laser kinetics program described has been constructed with considerable emphasis on flexibility and simplicity of usage for the user. In addition to the instructions for usage described in the present report, the FORTRAN source decks contain extensive internal COMMENT card documentation as well. Even synthesized subroutines which are generated by translation of the input reaction queue contain COMMENT card documentation. In addition to the laser kinetics synthesis and analysis code, an independent program for solution of the Boltzmann equation has been developed, and is also included in the present report. All of the programs and subroutines have been written in FORTRAN IV for Extended Fortran Compilation on the CDG 6000 and CYBER Series of computers (which use a 60-bit, 10-BCD display character) word. Extensive modifications may be required if these codes are to be executed on some other system.

The present programs were developed in support of experimental research projects for the KrF excimer laser. Therefore, input and output for analysis of a KrF system are used for illustration. Program listings are given in Vol. II of this report.



THEORETICAL MODELING OF MOLECULAR AND  
ELECTRON KINETIC PROCESSES

Volume I, II

ACCESSION for	
NTIS	<input checked="" type="checkbox"/>
DOC	<input type="checkbox"/>
UNANNOUNCED	<input type="checkbox"/>
JUSTIFICATION	<input type="checkbox"/>
BY	
DISTRIBUTION/AVAILABILITY CODES	
Dist.	
A	
ALL	
SPECIAL	

Contract Number:

N00014-78-C-0499  
613C:MAK

Principal Investigator:

Dr. William B. Lacina  
(213) 377-4811, Ext. 322

Name of Contractor:

NORTHROP Corporation  
Northrop Research and  
Technology Center  
One Research Park  
Palos Verdes Peninsula  
California 90274

Scientific Officer:

Director, Physics Program  
Physical Sciences Division  
Office of Naval Research  
Department of the Navy  
800 N. Quincy Street  
Arlington, Virginia 22217

Technical Monitor:

Dr. Robert Behringer  
Office of Naval Research  
Pasadena, California

Contract Period:

12 June 1978 - 15 Jan. 1979

Reproduction of this document in whole or in part is permitted  
for any purpose of the United States Government.

The views and conclusions contained in this document are those  
of the author and should not be interpreted as necessarily repre-  
senting the official policies, either expressed or implied, of the  
Office of Naval Research or of the United States Government.

THEORETICAL MODELING OF MOLECULAR AND  
ELECTRON KINETIC PROCESSES

Volume I

Theoretical Formulation of Analysis and  
Description of Computer Programs

TABLE OF CONTENTS

---

1.0	INTRODUCTION	1
2.0	SCOPE AND MATHEMATICAL STRUCTURE OF MODEL	8
2.1	Molecular Kinetics	9
2.2	Radiative Extraction	18
2.3	Electron Kinetics: Boltzmann Equation	23
2.4	External Driving Circuit and Ionization Sources	59
2.5	Conservation of Energy	62
3.0	COMPUTER PROGRAM DESCRIPTION	79
3.1	Program Structure and Flow Diagram	79
3.2	Input Data Description	89
3.3	Description of Subroutines	119
3.4	Boltzmann Analysis Program	140
3.5	Execution Control Cards	143
4.0	KrF LASER KINETICS: Illustrative Example of Program Synthesis and Execution	152
4.1	Molecular Kinetic Subroutine Generation	152
4.2	Execution of Analysis	158
4.3	Error Diagnostic Assistance	217
5.0	REFERENCES	232

---



## 1.0 INTRODUCTION

Northrop Research and Technology Center has been involved in a variety of research programs which have resulted in significant contributions to the development of high power laser technology as well as advances in the understanding of fundamental laser physics. Recent investigations have been focused on uv and visible laser concepts, with primary emphasis on the rare gas halide excimer systems such as  $\text{KrF}^{1-5}$ . In theoretical support of these experimental investigations, the present author has developed a comprehensive computer code which is sufficiently general that it would be of substantial future benefit for a wide variety of analytical studies of lasers, chemical kinetics, and electric discharge phenomena. This code,\* which contains far more generality and flexibility than any of its nominal competitors currently in existence, will be thoroughly described and documented in the present report in order to make it available to the general community.

During the past several years, there has been a continuing interest and extensive effort in theoretical modeling of laser kinetic phenomena. In support of research directed toward development of new laser concepts, construction of a computer analysis to model the fundamental physical mechanisms and microscopic kinetic processes can provide a valuable tool for understanding the laser operation and for optimizing its performance. Such a model is continuously refined as understanding of the laser reaction scheme evolves.

Exploratory research for the development of promising new laser systems is often a combination of art and science, and typically requires both ex-

---

\* This code was developed under internal IR&D funding, with partial support from the Advanced Research Projects Agency of the Department of Defense, monitored by the Office of Naval Research under contract N00014-76-C-1100.

perimental and theoretical understanding of several overlapping disciplines such as molecular spectroscopy and kinetics, electron kinetics and discharge circuitry, fluid dynamics, and laser radiative extraction. The first step in the discovery of a new laser system is the formulation of a conceptual mechanism of excitation and energy transfer for a set of candidate atomic and molecular species; usually, this is based initially upon only an intuitive or semiquantitative understanding of the spectroscopy and kinetic processes for the proposed system. Inspiration for a concept often originates from current fundamental research in the spectroscopy of highly excited states of known molecules or unfamiliar transient species, and from studies of collision dynamics and measurements of energy transfer reaction rates. If initial experimental investigations confirm that a hypothetical laser concept can be successfully realized, more detailed studies complemented by theoretical modeling and analysis are required in order to optimize laser performance and to formulate quantitative scaling laws for extrapolation to high power, efficiency, and volume. For this purpose, it is necessary to understand the kinetic and pumping processes which are responsible for the formation and quenching of the excited species. A theoretical model of the fundamental physical mechanisms, implemented by a computer code, is a useful asset for the development and optimization of a practical laser device.

The typical development of a laser kinetic model proceeds by constructing an analysis of a spatially uniform gain medium in a simple plane parallel resonator with an attempt to describe, as completely as possible, all of the coupled phenomena involving atomic and molecular kinetics, electron kinetics, discharge circuitry, optical radiative extraction, fluid dynamics, etc. which characterize the laser system. Although the goal of such an effort is to provide a reliable analytical tool for optimizing the development of a practical laser device, such a model may also be useful even when the laser may fail to accurately exhibit the predicted



behavior in all respects. In such a case, one may still be able to define parametric trends which suggest the necessary approach for optimization of the laser device. Even with an incomplete model, it is often possible to better understand the importance of microscopic processes or excited species, and/or to eliminate some unimportant factors from further investigation. In fact, evolution in the theoretical understanding of the fundamental physical mechanisms of the laser proceeds by just such a process in which the sensitivity of various rate constants is assessed, the dependence of observed output on various experimental parameters is determined, and the kinetic reaction scheme is modified to account for and to better explain the observed phenomena. Although such a model is continually refined as the understanding of the reaction scheme evolves, even preliminary predictions from the analysis may be sufficiently reliable to justify more extensive experimental effort, or to define and narrow the range of parameters or direction of approach.

The most important theoretical components of the model consist of the analysis of the fundamental physical mechanisms, and in particular, the refinement of the molecular kinetic reaction scheme and estimates of its rate constants. Simultaneously, attempts at more sophisticated description of related problems such as discharge stability, medium nonuniformity, optical extraction and resonator configuration, flow properties, and mode-medium interactions can be undertaken. In general, all of the latter refinements are concerned more with an improved description of effects which result from spatial inhomogeneity rather than with fundamental physical mechanisms, and are therefore most appropriate only in the final stages of development of a realistic engineering model. That is not to say that these effects are unimportant, for they often present practical limitations that make it difficult to attain the results predicted for an idealized homogeneous medium.

Therefore, the scope of the present work was to develop a coupled analysis of molecular kinetics, electron kinetics, electric discharge circuit, and optical radiative extraction, which form the fundamental basis for the description of the physics of an electrically excited laser system. The goal of any such model is to successfully predict, for a spatially uniform gain medium, the excited state population densities, gain and saturation parameters, power transfer and extraction rates, electrical power partitioning, optical conversion efficiency and specific power, optical output power and spectral distribution, etc.

In general, the type of model developed, the detail and approximations considered, the computational sophistication, the input/output flexibility of the computer code, etc., can vary considerably depending upon the specific problem and application. There is currently much needless duplication of effort devoted to laser kinetic modeling. For any specific laser concept, there is often a considerable overlap as well as a frequent lack of communication between competing investigators engaged in identical kinetic analyses. Furthermore, this overlap is even more extensive when one considers the work of those who have developed essentially the same analytical models for different systems which (although not identical) are nevertheless members of a broad class of electrically excited lasers for which a more generally applicable analysis could have been developed. These concurrently developed computer codes are rarely, if ever, documented or intended for distribution. Because they vary considerably in sophistication and approach, are generally written without regard for user-orientation, often lack flexibility in problem scope or have cumbersome input/output structure, and usually require extensive effort to modify them for application to new systems, they are essentially useless to anyone but their original authors. As a result, government agencies which fund such research often pay for the same product sever-



al times, and future programs cannot directly build upon or benefit from the previous work. It is impractical to construct a new computer code for the analysis of each new kinetic reaction scheme. If the necessity of computer programming were substantially eliminated by the availability of an applicable, user-oriented, existing computer code, a significant amount of time could be saved and allocated to more productive efforts to understand the physics of the laser system.

Recognition of the lack of a coherent and unified approach to the problem of laser kinetic modeling provided the inspiration to undertake the development of a generalized computer code which would be applicable to a broad class of transient, electrically excited laser systems. The present code automatically synthesizes, for an arbitrary reaction scheme, a completely self contained computer code for numerical solution of the coupled equations which describe the molecular kinetics, electron kinetics, external driving circuit, and optical radiative extraction. This code automatically generates its own subroutines for the analysis of molecular kinetics by translating symbolic reactions, provided as input, into computer-coded equations. Thus, for the most complicated reaction scheme containing an arbitrary number of kinetic collision processes and interacting species, it is possible to obtain the complete computer code required with virtually no effort. The automatically synthesized molecular kinetics subroutines are combined with a master executive program and all other required subroutines (e.g. for numerical solution of the Boltzmann transport equation) to form a completely self-contained coupled analysis based upon the specified reaction scheme.

With appropriate modifications, this code can be easily adapted to the analysis of related problems in various fields which involve studies of chemical kinetics. Its internal subroutines for numerical solution of

the Boltzmann equation can be employed for the analysis of transport properties of electrical discharges, and a separate program developed for this purpose will be described in Sec. 3.4 (cf. Vol. II for listing).

The present computer code is completely user-oriented, and for a very broad class of transient, electrically excited laser systems, it completely eliminates the necessity for the laborious task of constructing new computer codes. It will do, automatically, work that would require several months if done manually, and it will provide an input/output flexibility for the synthesized analysis surpassing that which typically characterizes existing codes that have been developed for specific systems.

It was felt that documentation and dissemination of this computer code to those engaged in laser kinetic modeling would provide substantial benefit and economy by the elimination of needless repetition and duplication of effort. It has been the intent of the author that every effort be made to maximize the flexibility and simplicity of usage of the code, and that the description of the analysis and computational structure be sufficiently clear and detailed that others shall be able to modify and/or extend the analysis as they require. The objective has been to reduce mechanical programming considerations to a minimum, and to provide the user with (limited) diagnostic assistance as well as some protection by automatic exit if specified error conditions are encountered during execution.

The present code has been written in an extended version of FORTRAN IV with syntax and conventions compatible with the CDC 6600 computer. It makes extensive use of a 60-bit, 10-BCD character word size, as well as various special features permitted by the current CDC FTN compiler, so considerable effort may be required if it should be necessary to adapt it to execute on other machines. However, because the CDC 6600 cur-



rently enjoys widespread usage for scientific applications at government, industrial, and university research laboratories, it is anticipated that the code will be suitable for the majority of potential users. In order that the program may be more easily modified or extended, the source decks have been extensively documented with internal COMMENT cards. Furthermore, even the synthesized subroutines are generated with internal COMMENT card documentation to make them completely readable and understandable. The synthesized code is a complete and self-contained FORTRAN source program.

Obviously, because this code has been developed as a research tool in support of current experimental laser development programs, it is not possible to guarantee that it will perform perfectly under all conditions to which it may be applied, although every effort has been taken to insure that it do so. Even programs which are free of logical or programming errors can fail for reasons of numerical ill-conditioning, convergence difficulties, computational instabilities, accidental division by zero, etc. Because the present code was developed primarily in support of KrF laser research, the illustrative examples to be presented in subsequent sections shall apply to that system.

It has been said that "All computer programs must be assumed to contain bugs until proven otherwise, which is impossible." Users who discover suspected "bugs" in the present analysis are encouraged to communicate them to the author who, in turn, will attempt to offer assistance to users when necessary. It is hoped that investigators who benefit from the availability of this code will make appropriate acknowledgments of its usage in the footnotes or references of their published papers, conference presentations, or reports.

## 2.0 SCOPE AND MATHEMATICAL STRUCTURE OF THE MODEL

The scope of the present work was the development of a comprehensive and reasonably general computer analysis applicable to a broad class of transient, electrically excited laser systems. The theoretical model is formulated, for a spatially homogeneous medium, in terms of the coupled set of equations which describe the molecular kinetics, electron kinetics, external discharge circuit, and optical radiative extraction. For each new laser kinetic scheme, the equations which define the molecular and electron kinetics are different, and the main advantage of the present computer code is that it generates the required analysis automatically by synthesizing the necessary subroutines. It is especially useful for systems characterized by complicated, but relatively unsystematic, kinetic reaction schemes. Its most appropriate application is to uv and visible laser systems which involve excitation, energy transfer, and stimulated emission from electronic states of atoms and molecules.

For infrared laser such as CO, CO<sub>2</sub>, HF, etc., the mechanism of pumping, energy transfer, and radiative emission involves the excited vibrational levels of the ground electronic state, and for these lasers, the present approach (with modifications) would be relatively inefficient, if not totally inadequate. For the infrared laser systems, a more complicated treatment of radiation must often be included to allow for possible absorption and emission for several vibrational-rotational transitions, and there are strong temperature effects in the vibrational kinetics as well as in the radiative processes. In its present form, the analysis does not include effects of changes in the molecular temperature, and there is no provision for temperature dependent parameters. For such problems, the construction of a more specialized analysis which explicitly recognizes the systematic structure of the vibrational-rotational level interactions,

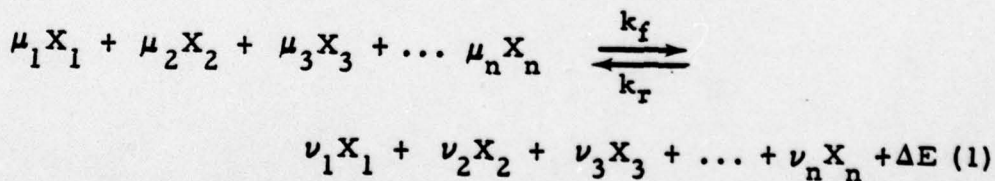


and which can most easily incorporate temperature dependent effects or other unique features, would probably be more suitable than attempts to modify, extend, and apply the present program. It is, of course, anticipated that there will be situations for which extensions or modifications of the present code, or of the subroutines which it synthesizes, will be the optimum approach.

The components of the present model, labeled with some brief descriptive remarks, are summarized in Fig. 2.1. From the more detailed discussion of the physics to be given below, it should become more apparent for which problems the present analysis is most applicable. A discussion of the limitations, approximations, numerical techniques, and range of applicability of the analysis will be provided.

## 2.1 Molecular Kinetics

The molecular kinetics are described by the master equation for the population densities of all the atomic and molecular species present in the electrically excited gas mixture, including electrons, ions, neutrals, excited states, excimers, etc. For a given set of reactions, the formal construction of the master equation for the population densities is illustrated in Fig. 2.2. If the species involved are  $X_1, X_2, X_3, \dots, X_n$ , any reaction in the molecular kinetic scheme can be written



where  $k_f$  and  $k_r$  are forward and reverse rate constants ( $s^{-1}$ ,  $cm^3/s$ ,  $cm^6/s$ , etc.), and  $\mu_i$  and  $\nu_i$  are (nonnegative) integer coefficients (most of which are zero or one). The conservation of energy in Eq. (1) gives

## COUPLED LASER KINETICS ANALYSIS

- **MOLECULAR KINETICS**

Master Equation for population densities of all atomic and molecular species (electrons, ions, neutrals, excited states, excimers, etc. ).

- **ELECTRON KINETICS**

Boltzmann transport equation for the electron energy distribution to determine plasma parameters, electrical excitation rates, power partitioning, and discharge efficiency.

- **CIRCUIT ANALYSIS**

External circuit equations to describe the electrical power loading in a low impedance gas discharge, whose conductivity is function of  $t$ .

- **OPTICAL EXTRACTION**

Oscillator analysis, formulated in terms of intracavity photon density, with transient build-up of laser mode from spontaneous emission and subsequent relaxation to quasi-steady condition with gain at threshold.

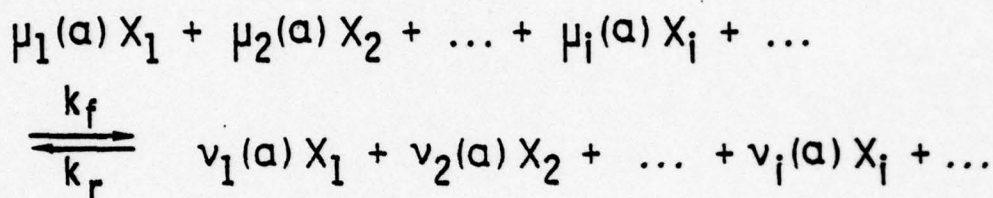
**Fig. 2.1: Basic components for the theoretical analysis of an electrically excited laser system.**



## MOLECULAR KINETICS

Species  $i$ :  $X_1, X_2, X_3, \dots, X_i, \dots, X_n$

Reactions  $\alpha$ :



Rate:

$$R(\alpha) = k_f(\alpha) [X_1]^{\mu_1(\alpha)} [X_2]^{\mu_2(\alpha)} \dots [X_i]^{\mu_i(\alpha)} \dots$$

$$- k_r(\alpha) [X_1]^{\nu_1(\alpha)} [X_2]^{\nu_2(\alpha)} \dots [X_i]^{\nu_i(\alpha)} \dots$$

Molecular Kinetics Master Equation:

$$\frac{d[X_i]}{dt} = \sum_{\alpha} R(\alpha) [\nu_i(\alpha) - \mu_i(\alpha)]$$

Fig. 2.3: Construction of the molecular kinetics master equation for the rates of change of population densities for an arbitrary number of interacting species in a general reaction scheme with collision processes  $\alpha$ .

an expression for the net energy change  $\Delta E$ :

$$\sum_i \mu_i E_i = \sum_i \nu_i E_i + \Delta E$$

The net rate per unit volume ( $\text{cm}^{-3} \text{s}^{-1}$ )  $R$  for the forward and reverse reaction of Eq. (1) is given by

$$R = k_f [X_1]^{\mu_1} [X_2]^{\mu_2} [X_3]^{\mu_3} \dots [X_n]^{\mu_n} - k_r [X_1]^{\nu_1} [X_2]^{\nu_2} [X_3]^{\nu_3} \dots [X_n]^{\nu_n} \quad (2)$$

where  $[X_i]$  is the population density ( $\text{cm}^{-3}$ ) of the  $i$ th species  $X_i$ . The contribution that such a reaction makes to the rate of production (or loss) of the  $i$ th species is given by

$$d/dt [X_i] = (\nu_i - \mu_i) R. \quad (3)$$

Thus, for an arbitrary reaction scheme containing several collision processes (labeled by  $\alpha$ ), the complete master equation becomes

$$d/dt [X_i] = \sum_{\alpha} [\nu_i(\alpha) - \mu_i(\alpha)] R(\alpha) \quad (4)$$

If Eq. (4) is multiplied by the energy  $E_i$  of the  $i$ th species  $X_i$ , and then summed over  $i$ , an equation for the conservation of energy (in terms of power balance) is obtained:

$$d/dt \sum_i E_i [X_i] = - \sum_{\alpha} R(\alpha) \Delta E(\alpha) \quad (5)$$

where

$$\Delta E(\alpha) = \sum_i [\mu_i(\alpha) - \nu_i(\alpha)] E_i \quad (6)$$

is the net energy change for reaction  $\alpha$ . The sum over  $i$  in Eq. (5), (6) implicitly excludes secondary electrons  $e^-(u)$ , whose contribution to the total power conservation equation must be expressed as an integration over the continuum of electron energies  $u$ . The formulation of electrical power balance will be given in Sec. 2.3 below, where analysis of electron kinetics based upon the Boltzmann equation for the electron energy distribution is discussed. The total power balance equation will be developed in Sec. 2.5, where the physical interpretation of various terms corresponding to optical, electrical, and kinetic heating mechanisms will be given.

We may, for convenience, formally define the parameter  $E_i$  to be zero for secondary electrons, so that their exclusion from the sums in Eq. (5) and (6) does not need to be made explicit. To be consistent, it is then necessary (for the purpose of Eq. (5)) to suppress the energy dependence denoting the continuum of electron species  $e^-(u)$ . In doing this, it should be emphasized that the parameter  $E_i = 0$  for the single species "electron" has no physical significance, and that the power balance relation (5) must ultimately be supplemented with the contributions originating from the electrical processes.

To write the subroutines which define the molecular kinetics for a complicated reaction scheme is, in general, a difficult and time-consuming



task, and the resulting computer program would have little flexibility for analysis of any system except those in a very limited class. (For example, there have been as many as  $\sim 80$  reactions considered to be of possible importance for modeling KrF laser kinetics.) Furthermore, as understanding of a laser reaction scheme evolves, addition of new reactions (or deletion of old ones) may be continually required, in addition to making simple updated estimates of the rate constants for the reactions retained. Thus, such a code would itself have to be modified in a continuing manner, rather than merely executed with revised input values for the rate constants.

Therefore, in order to provide a more powerful analytical capability applicable to a wide class of problems, a generalized code has been developed which automatically synthesizes the coupled analysis described in Fig. 2.1 for an arbitrary reaction scheme. The input to this code is a sequence of reactions and (initial) estimates of rate constants. The syntax for the reactions is very flexible, with a free format that accepts the reaction just as it would normally be written. The content of each reaction is analyzed, and the appearance of each new species is recognized. The syntax of each reaction is subjected to numerous tests to detect errors. If the reaction is determined to be acceptable, it is decomposed and translated into appropriate computer-coded expressions in order to generate synthetically the required subroutines. Program generation and execution are protected by diagnostic assistance and automatic exit (according to input requests) if specified error conditions are encountered. A more detailed discussion of the structure of the code will be given in a subsequent section devoted specifically to program description.

Fig. 2.3 presents a schematic flow diagram of the present approach. The rate constants initially assumed in the generation of the program

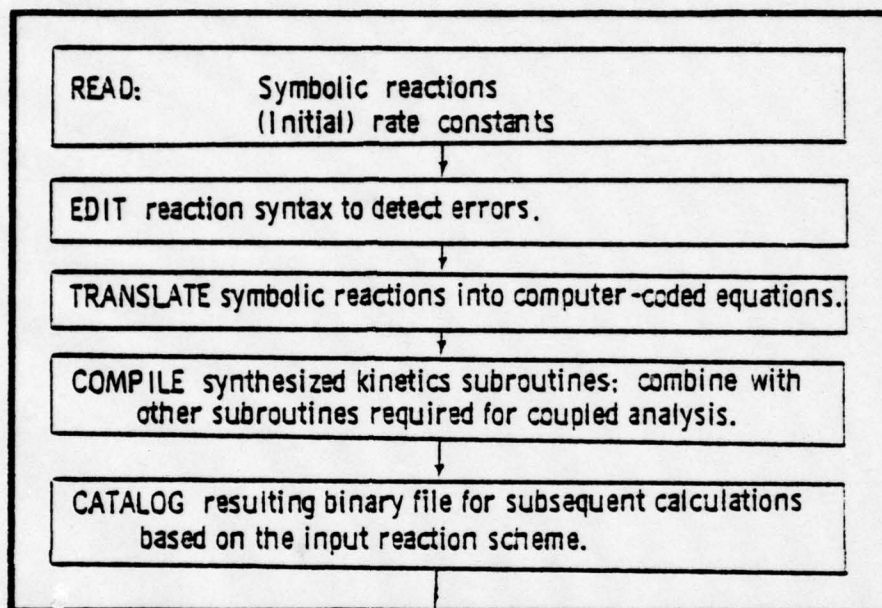
can be changed in the subsequent execution, if desired. The main purpose of the rate constants in the initial input deck is to define whether the forward and/or reverse process is to be included in the rate expressions. If, during program generation, a zero rate constant is encountered for any process (other than secondary electron collisions), no translation of the forward (or backward) term occurs in the synthesized subroutines. Of course, if the correct values of the rate constants are known, they may be entered for once and for all in the original input deck. As Fig. 2.3 indicates, the synthesized molecular kinetics subroutines are automatically combined with the master executive program and all other required subroutines to form a completely self-contained coupled analysis based upon the specified reaction scheme. The section enclosed in the upper box in Fig. 2.3 is required only when a new reaction scheme is introduced and generation of a new program is required. For all subsequent calculations based upon the given reaction scheme, the initial conditions, experimental parameters, rate modifications (if any), and I/O and control parameters are entered, and the complete code constructed in the upper box is executed. That is, only the lower section of Fig. 2.3 is involved thereafter.

There are several obvious advantages to this approach. First of all, there is the simplicity of automation and the minimization of the possibility of error in the writing of complicated subroutines. Secondly, the program diagnoses error conditions in the reaction syntax which may not have been noticeable or which may have been overlooked. For example, duplicate reactions are detected (even when written backwards), charge particle and heavy particle conservation is insured, detail balance relations for binary collision processes are enforced, and miscellaneous other error conditions are detected. Secondary electron collision processes are recognized and properly coupled to the electron kine-



## GENERALIZED SYNTHESIS LASER KINETICS CODE

### Synthesis :



### Analysis :

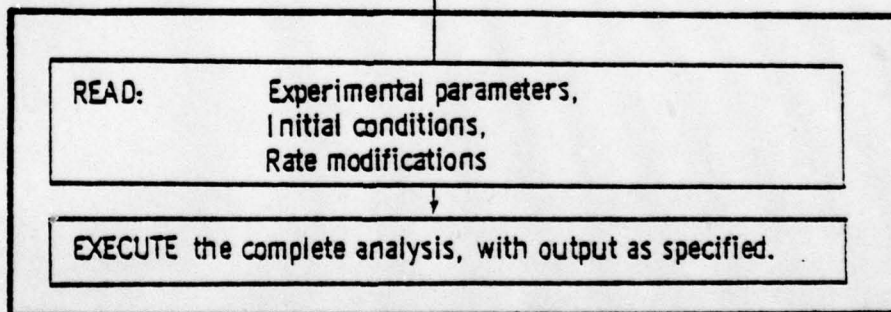


Fig. 2.3: Schematic flow diagram of the functional structure of the laser kinetics code. A complete FORTRAN source program is synthesized by translation of symbolic reactions into computer-coded equations. Execution of the analysis occurs in the lower box.

tics analysis, except for cases without electric discharge (e.g.  $e^-$ -beam excitation only), in which case their rate constants can be defined by input. Finally, the subroutines are constructed in such a way that null operations (multiplications or additions involving zero) are completely eliminated (if no rate constant is provided for the forward or reverse process, no translation of the corresponding term occurs), and in such a way as to optimize computational efficiency (repetitious or unnecessary multiplications are minimized). Even for relatively simple problems with uncomplicated molecular kinetic reaction schemes, the availability of a program which can automatically provide the investigator with a user-oriented code with good I/O flexibility and simplicity of usage is of obvious advantage.

It is usually the case that the rate constants involved in molecular kinetic reaction schemes can vary over several orders of magnitude, and therefore, the resulting master equation (4) often becomes a "stiff" system of differential equations. Therefore, the approach which has been taken for integration of these equations is to employ a multistep technique developed by Gear<sup>6</sup>. This method automatically adjusts the integration step size as the solution proceeds, in such a way that required accuracy conditions are maintained. The Gear method requires subroutines not only for the rates of change  $\dot{n}_i = d[X_i]/dt$  of the population densities, but also for the Jacobian,  $\delta \dot{n}_i / \delta n_j$ , as a function of time. Because numerical evaluation of the Jacobian is not generally satisfactory, it is necessary to generate both such subroutines symbolically in the synthesis section of the program, where the reaction scheme is decomposed and translated into computer-coded equations.

The entry of control parameters, experimental parameters, revised rate constants, initial conditions, output requests, etc., is quite flexible, and

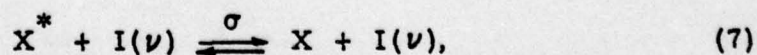


permits the code to be executed for a variety of situations of interest. For example, rate constants for secondary electron collisions are obtained self-consistently from the coupled Boltzmann analysis for the case of an electric discharge. For the case of  $e^-$ -beam excitation only, these rate constants default automatically to zero, but can be specified by input, if desired. This is useful for entering thermal (i.e. room temperature) values for electron recombination or attachment processes, for example. Thus, the same general code can be used for both discharge or  $e^-$ -beam excitation conditions. Likewise, it is possible to apply it to either an oscillator or amplifier analysis.

The integration of the coupled set of equations over the total specified pulse length is carried out with the Gear technique, which automatically adjusts the step size to maintain accuracy and stability. However, the total pulse length is divided into a finite number (nominally 50) of subintervals, at which time the electron kinetics are updated and a variety of output option requests can be supplied.

## 2.2 Radiative Extraction

The basic features of the radiation analysis are summarized in Fig. 2.4. Because considerable simplification can be achieved by neglecting complications associated with a rigorous description of the optical fields in a realistic resonator configuration, a spatially homogeneous medium is assumed, with an optical resonator formed by two plane parallel mirrors. The net amplification of the intracavity radiation intensity  $I(\nu)$  from the stimulated emission and absorption process





## OPTICAL EXTRACTION

- Spatially uniform intracavity optical fields.
- Plane parallel optical resonator (100% R), separation  $L_c$ .
- Spatially uniform gain medium of length  $L_g$ .
- Distributed output coupling and loss ( $\gamma$ ) coefficients.
- Cavity threshold gain coefficient:

$$a_{th} = [\gamma + (1/2) \ln(1/R)] / L_g$$

- Buildup of optical fields:

Spontaneous emission in solid angle  $\Omega$  defined by output coupling aperture and resonator length:  $A/L_c^2$ .

Amplification from stimulated emission, offset by the intracavity absorption and output coupling losses.

- Formulation in terms of intracavity photon density:

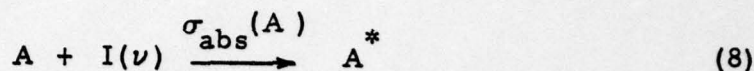
$$n_{ph} = 1/chv$$

$$dn_{ph}(t)/dt = (L_g/L_c) [c(a(t) - a_{th}) n_{ph}(t) + \frac{N}{\tau} \frac{\Omega}{4\pi}]$$

- Cavity buildup time:  $t_c = L_c/L_g a_{th} c$

**Fig. 2.4:** Basic formulation of radiative extraction in terms of intracavity photon number density, with buildup of optical fields from spontaneous emission.

corresponding to the laser transition from an excited state  $X^*$  to a lower state  $X$ , as well as by absorption processes such as



can be written

$$dI(t)/dt = c[\alpha(t) - \alpha_{\text{th}}]I(t), \quad (9)$$

where  $\alpha(t)$  is the instantaneous net gain coefficient in the medium (i.e. active gain offset by absorption),

$$\alpha(t) = [N^*(t) - N(t)]\sigma - \sum_A n_A(t)\sigma_{\text{abs}}(A), \quad (10)$$

and  $\alpha_{\text{th}}$  is the cavity threshold loss coefficient. Actually, (9) applies only to the situation where the cavity length  $L_c$  and the gain length  $L_g$  of the active medium are equal; if they are unequal, it must be modified to read

$$dI(t)/dt = (L_g/L_c)c[\alpha(t) - \alpha_{\text{th}}]I(t) \quad (11)$$

The factor  $L_g/L_c$  has the significance of a contraction in the radiative time scale to account for the fact that during a round trip cavity time, the gain medium is encountered during only a fraction ( $L_g/L_c$ ) of that time. Equivalently, if the gain medium were considered to be distributed uniformly over the entire cavity length  $L_c$  (rather than over the actual gain length  $L_g$ ), then the actual gain would have to be reduced by the factor  $L_g/L_c$  to produce an equivalent round trip amplification. It should also be noted that  $L_g/L_c$  is the ratio of the active gain volume to the optical cavity volume, and therefore this factor logically appears in the formulation of the equation for conservation of power density.

It is convenient to treat stimulated emission and absorption processes in a manner parallel to that for kinetic collision reactions. Therefore, the equation for radiative extraction will be formulated in terms of the photon number density in the cavity, defined by

$$n_{ph} = I / ch\nu. \quad (12)$$

This will also facilitate the incorporation of spontaneous emission as a source term for the buildup of the optical fields from noise. The equation for the photon number density includes the source term from spontaneous emission, amplification from stimulated emission, and losses from output coupling and/or intracavity absorption:

$$dn_{ph}/dt = (L_g/L_c) \left[ N^*/\tau (\Omega/4\pi) + c[\alpha(t) - \alpha_{th}] n_{ph} \right]. \quad (13)$$

$\alpha_{th} = [\gamma + (1/2)\ln(1/R)]/L_g$  is the threshold loss coefficient expressed in terms of the intracavity loss per pass  $\gamma$  and the output coupling reflectivity  $R$ ,  $(\Omega/4\pi)$  is the fractional part of the total spontaneous emission which builds up the laser mode (taken to be the solid angle  $\Omega$  subtended by the output coupling mirror viewed from the opposite end of the cavity), and  $\alpha(t)$  is the instantaneous net gain coefficient in the medium defined by Eq. (10).

Note that transient effects are included in the present description of the radiation field. Although a steady state oscillation condition (i.e., for which the gain and loss coefficients are equal) will typically occur during the time scales of interest, such a condition is not an a priori assumption of the present analysis. This approach allows the radiation intensity to be described for situations where pumping and kinetic times are comparable to the cavity decay time,



$$t_c = L_c / (L_g c \alpha_{th}). \quad (14)$$

For such situations, gain relaxation effects can be observed in which the net gain initially overshoots the cavity threshold and subsequently decays to the steady state gain condition,  $\alpha(t) = \alpha_{th}$ . Under conditions of high pumping the overshoot can be significant, since the stimulated emission from the medium occurs under conditions of high gain.

When formulated in terms of the intracavity photon density, the radiation equations can be included in a unified way with the other kinetic collision processes of the laser reaction scheme. For example, the stimulated emission process (7) can be described by the equations

$$dN^*/dt = -k_f N^* n_{ph} + k_r N n_{ph} = k(N - N^*) n_{ph} \quad (15.1)$$

$$dN/dt = -dN^*/dt \quad (15.2)$$

$$dn_{ph}/dt = (L_g/L_c) k(N^* - N) n_{ph}, \quad (15.3)$$

where  $k_f = k_r = k = c\sigma$ , and  $\sigma$  = stimulated emission (and absorption) cross section ( $\text{cm}^2$ ). Likewise, the contribution of reaction (8) to the photon field is

$$dn_{ph}/dt = - (L_g/L_c) k_{abs}(A) n_A(t) n_{ph}, \quad (16)$$

where  $k_{abs}(A) = c\sigma_{abs}(A)$  is the rate constant for absorption ( $\text{cm}^3/\text{s}$ ). Although minor modifications are required to incorporate the factors  $(\Omega/4\pi)$  and  $(L_g/L_c)$  and the term  $-c\alpha_{th} n_{ph}$  in Eq.(13), the similarity in structure of Eq. (3), (15), and (16) permits the radiation field (photons) to be treated on an equal basis with the other molecular species in the construction of the master equation described earlier.

### 2.3 Electron Kinetics: Boltzmann Equation

The present analysis of an electrically excited laser medium incorporates a completely coupled treatment of molecular and electron kinetics. The electron kinetics analysis is based upon the assumption that the plasma has attained a quasisteady state on the time scales of electrical pumping and inelastic secondary electron collision processes, so that the electron energy distribution function  $f(u)$  can be obtained from solution of the time-independent Boltzmann equation as a function of gas mixture and the instantaneous values of  $E/N$  and excited state population densities. The present analysis includes electron-molecule inelastic collisions, elastic electron-molecule momentum transfer collisions (with recoil), electron-electron (i.e., Coulomb) scattering, and excitation from an applied (dc) electric field as well as source terms for electron creation (and resulting energy deposition) from an external  $e^-$ -beam. Superelastic electron collisions (i.e., reverse processes in which electrons gain energy by collisions with excited molecular species) are important in situations with high excited state population densities, and are included in both the molecular and plasma kinetic equations. Electron-electron scattering effects, which can become important under conditions of high fractional ionization, are included. From the solution of the Boltzmann equation, all of the electron transport coefficients, elastic and inelastic secondary electron collision rates, electrical power partitioning, etc., can be obtained.

One of the unique features of the present analysis is a self-consistent treatment of secondary ionization and attachment phenomena by retention of a quasisteady term proportional to  $dn_e/dt$  to properly account for transient plasma effects that occur on the time scale of the molecular and electron kinetic processes. The usual formulation of the time-



## ELECTRON KINETICS ANALYSIS

- Electron Energy Distribution  $f_0(u)$ : Numerical solution of the Boltzmann transport equation.
- Quasisteady state approximation: the term proportional to  $dn_e/dt$  is retained to describe situations for which there is a net creation (or loss) of electrons.
- Source term included to describe external ionization (e.g., electron beam or photoionization):

$$S(u) = S_0 \delta(u) + S_b(u).$$

$S_0$  term provides for the external creation of electrons at zero energy.

- Momentum transfer with recoil; elastic heating of the molecular gas.
- Binary inelastic electron - molecule collision processes included; e.g.,  
Vibrational Excitation, Electronic Excitation, Secondary Ionization, Attachment, Recombination, Dissociation, etc.
- Electrons created by secondary ionization assumed to be at zero energy and included in a source term  $\sim \gamma_i \delta(u)$ .
- Electron-electron collisions (Coulomb scattering) are included (important for high fractional ionization,  $\geq 10^{-5}$ ).
- Charged particle interactions between electrons and heavy ions neglected.
- Superelastic collisions, important for excited gas mixtures, are included.
- Electrical parameters, calculated as a function of  $E/N$ , gas mixture, and the excited state population densities:

Mobility, Drift Velocity, Average Energy, Effective Temperature, Characteristic Energy, Diffusion Coefficient, Plasma Conductivity, Discharge Current Density, Power Densities.

Forward (and reverse) secondary electron excitation rates.

Fractional partitioning of electrical input power into rate of energy storage and all elastic and inelastic scattering mechanisms.

**Fig. 2.5: Summary of features of the electron kinetics analysis.**

independent Boltzmann equation assumes that the inelastic processes include only binary electron-molecule collisions for which there is no net creation or loss of secondary electrons. When creation or loss of electrons occurs by secondary ionization, attachment, recombination, external sources of ionization, etc., it is necessary to retain the term proportional to  $dn_e/dt$  in the time-dependent Boltzmann equation in order to properly describe the conservation of electron density. If the electron energy distribution  $f(u)$  were known, the rates of secondary ionization, attachment, recombination, etc. could all be calculated and  $dn_e/dt$  could be determined. However,  $dn_e/dt$  occurs as a parameter in the Boltzmann equation, and in order to calculate  $f(u)$ , its value must be known. Therefore, an iterative approach was developed for a self-consistent determination of  $dn_e/dt$ . The numerical techniques for solution of the Boltzmann equation will be described in detail later.

The basic features of the electron kinetics analysis are summarized in Fig. 2.5. The scope of the present analysis is considered to be quite comprehensive. In addition to the fact that the present formulation includes more refinements than many of the Boltzmann analyses currently in usage, the computer subroutine for its numerical implementation is quite flexible and computationally efficient.

#### Theoretical Formulation

In general, the electron energy distribution function for the gas mixtures and relatively low  $E/N$  values typical of electric discharge lasers is highly non-Maxwellian. The increasing availability of extensive experimental cross section data for elastic and inelastic electron collision processes for many gases of interest often makes it possible to obtain a quantitative analysis of electron kinetics by direct numerical solution of the Boltzmann equation. If there is no net creation or loss of electrons by external source, secondary ionization, recombination, or at-



tachment, the electron velocity distribution  $f(\vec{v})$  for a multicomponent gas in an external electric field  $\vec{E}(\vec{r}, t)$  satisfies the Boltzmann transport equation,

$$\left[ \partial/\partial t + \vec{v} \cdot \vec{\nabla}_{\vec{r}} - (e/m) \vec{E}(\vec{r}, t) \cdot \vec{\nabla}_{\vec{v}} \right] f(\vec{v}, \vec{r}, t) = \delta f / \delta t \Big|_c \quad (17)$$

where the collision term on the right hand side includes the effects of all elastic and inelastic scattering processes. A detailed discussion of the Boltzmann transport equation can be found in works by Holstein,<sup>7</sup> Allis<sup>8</sup>, Schkarofsky et al<sup>9</sup>, Frost and Phelps<sup>10</sup>, Carleton and Megill<sup>11</sup>, and Englehardt et al<sup>12, 13</sup>. Various approximations and techniques for its numerical solution and application to the analysis of electric discharge gas lasers have been discussed by Nighan et al<sup>14</sup>, Rockwood<sup>15</sup>, Hancock et al<sup>16</sup>, Elliott et al<sup>17</sup>, Morgan and Fisher<sup>18</sup>, Lowke et al<sup>19</sup>, Lacina<sup>20</sup>, and others. The present approach is based upon extensions and generalizations of earlier work<sup>20</sup> related to analysis of CO kinetics.

At the gas densities of interest for laser operation, elastic and inelastic electron-molecule collision frequencies are so high, relative to those for molecular kinetic processes, that the electron distribution function can be assumed to have adjusted "instantaneously" on the time scales over which the excited state population densities are evolving. It follows, therefore, that the first term of Eq. (17) containing the partial time derivative can be discarded if the electric field  $\vec{E}(\vec{r}, t)$  is assumed to be dc or slowly varying. For a spatially uniform field, it is similarly possible to neglect the second term, since the mean free path (which is related to the elastic collision cross section and molecular density) is typically small compared to the discharge dimensions. Thus, the Boltzmann equation (17) becomes

$$- (e/m) \vec{E} \cdot \vec{\nabla}_{\vec{v}} f(\vec{v}) = \delta f / \delta t \Big|_c. \quad (18)$$



The usual approach for solving this equation begins with an expansion of  $f(\vec{v})$  into Legendre polynomials,

$$f(\vec{v}) = f_0(v) + (\vec{v}/v) \cdot \vec{f}_1(v) + [3\vec{v}\vec{v}/v^2 - \vec{1}]:\vec{f}_2(v) + \dots \quad (19)$$

( $\vec{1}$  and  $\vec{f}_2$  represent dyadic quantities.) Usually,  $f$  can be well approximated using only the first two terms,

$$f(\vec{v}) = f_0(v) + (\vec{v}/v) \cdot \vec{f}_1(v). \quad (20)$$

Physically, the justification of a two-term approximation is related to assumptions about the degree of anisotropy to be expected for the velocity distribution. If the electric field is small enough that the directed speed of the electrons (as measured by their drift velocity) is much less than their random thermal velocities, the small first order perturbation  $\hat{v} \cdot \vec{f}_1$  from an isotropic distribution  $f_0(v)$  should be a good approximation. For high values of  $E/N$  characteristic of self-sustained discharges and for certain gases, it has been speculated<sup>21</sup> that the  $\vec{f}_2$  term may be comparable to the  $\vec{f}_1$  term, although no analysis has yet been undertaken to include these higher order terms quantitatively. Retention of more than the first two terms would require knowledge of angular (i. e. differential scattering) cross section data, which is not generally available. Typical experimental data gives only integrated cross sections (over all angles) as a function of the electron energy. Some of the available data in the literature has been determined indirectly by fitting measured transport coefficients to synthetic cross sections, using a numerical Boltzmann analysis based upon the two-term expansion (20) of  $f(\vec{v})$ . Thus, consistent use of that data would require that the electron kinetics calculations be based upon the two-term approximation. For values of  $E/N$  typical of  $e^-$ -beam sustained discharges, this approach is justified, and it is numerically much simpler than would be the case if angular calculations were required.

In the expansion (19),  $f_0(v)$ ,  $\vec{f}_1(v)$ ,  $\vec{f}_2(v)$ , ... are functions only of the magnitude  $v = |\vec{v}|$ , since all of the angular dependence has been put explicitly into the spherical harmonic coefficients  $\hat{v}$ ,  $(3\hat{v}\hat{v} - \vec{1})$ , ... etc. It can easily be verified that

$$\nabla_v f(\vec{v}) = \frac{1}{3v^2} (d/dv)(v^2 \vec{f}_1) + (df_0/dv)\hat{v} + (v/3)(d/dv)(v \vec{f}_1) \cdot (3\hat{v}\hat{v} - \vec{1}) + \dots \quad (21)$$

where  $\nabla_v f(\vec{v})$  has been separated into spherical harmonic terms which have  $\ell = 0, 1, 2$  symmetry, respectively. If (21) is substituted into (18) and separated into scalar and vector parts (which corresponds to multiplying by 1 or  $\hat{v}$  and integrating over the spherical solid angle  $\Omega_v$ ), the following equations result:

$$- (e\vec{E}/3mv^2) \cdot (d/dv)(v^2 \vec{f}_1) = \delta f_0 / \delta t \Big|_c \quad (22.1)$$

$$- (e\vec{E}/m)(df_0/dv) = \delta \vec{f}_1 / \delta t \Big|_c \quad (22.2)$$

The most important physical mechanism for reducing the asymmetry in the distribution function is electron-molecule momentum transfer collisions. The collisional rate of change of  $\vec{f}_1$  can be approximated by<sup>9</sup>

$$\delta \vec{f}_1 / \delta t \Big|_c = - \sum_X \nu_m^X(v) \vec{f}_1, \quad (23)$$

where  $\nu_m^X(v) = N_X v Q_m^X(v)$  is the momentum transfer collision frequency for molecules  $X$  in terms of the population density  $N_X$  and momentum transfer cross section  $Q_m^X(v)$ . In terms of the electron energy

$$u = mv^2/2e \quad (24)$$

(with  $u$  in units of eV,  $e = 1.602 \cdot 10^{-12}$  erg/eV =  $1.602 \cdot 10^{-19}$  J/eV), the

equation for  $f_0(u)$  becomes, after manipulation of Eq. (22) and (23),

$$-(E^2/3) d/du \left[ \frac{u}{\sum_X N_X Q_m^X(u)} df_0(u)/du \right] = \frac{mv}{2e} \frac{\delta f_0}{\delta t} \Big|_c. \quad (25)$$

Expressions for the collision term  $\delta f_0 / \delta t \Big|_c$  on the right hand side of Eq. (25) have been derived by Holstein<sup>7</sup>, Allis<sup>8</sup>, Schkarofsky et al<sup>9</sup>, Frost and Phelps<sup>10</sup>, and numerous others. It shall not be the purpose of the present discussion to repeat these extensive and rigorous derivations here.

However, it may be useful at least to motivate the form of the results for inelastic binary collisions characterized by an isotropic scattering cross section. For an inelastic scattering process, the collision term is defined simply as the net flux of electrons scattered into, and out of, a region  $[\vec{v}, \vec{v} + \Delta\vec{v}]$  of velocity space. The electrons scattered into  $[\vec{v}, \vec{v} + \Delta\vec{v}]$  originate from all volume elements  $[\vec{v}', \vec{v}' + \Delta\vec{v}']$  for which energy is conserved:

$$(1/2)mv'^2 = (1/2)mv^2 + eu_0 \quad (26.1)$$

or,

$$u' = u + u_0, \quad (26.2)$$

where  $u_0$  is the inelastic energy loss (eV) for the scattering process, and Eq. (24) was used. Under the assumption of isotropic scattering, Eq. (26) uniquely defines  $\Delta\vec{v}'$  for an arbitrary choice of  $\vec{v}$  and  $\Delta\vec{v}$ , for we can set  $\Delta\vec{v} \sim v^2 \Delta v$ ,  $\Delta\vec{v}' \sim v'^2 \Delta v'$ , and invoke Eq. (26) to obtain  $\Delta v' / \Delta v = v / v'$ . Therefore, it follows that



$$\Delta \vec{v}' = (v'/v) \Delta \vec{v}. \quad (27)$$

The rate ( $\text{cm}^{-3} \text{s}^{-1}$ ) at which electrons are scattered out of  $[\vec{v}', \vec{v}' + \Delta \vec{v}']$  is given by  $f(\vec{v}') \Delta \vec{v}' N v' Q(v')$ , where  $Q(v')$  is the scattering cross section and  $N$  is the neutral molecule particle density. Recall that  $f(\vec{v}') \Delta \vec{v}'$  represents the spatial density of electrons ( $\text{cm}^{-3}$ ) in the velocity region  $[\vec{v}', \vec{v}' + \Delta \vec{v}']$ , and that  $N v' Q(v')$  has the significance of collision frequency ( $\text{s}^{-1}$ ). In order to obtain an expression for the total flux of electrons scattered into  $[\vec{v}, \vec{v} + \Delta \vec{v}]$  from  $[\vec{v}', \vec{v}' + \Delta \vec{v}']$ , it is necessary to sum the contributions from all velocities  $\vec{v}'$  which satisfy the conservation of energy condition. The required "sum" over the continuum of velocities  $\vec{v}'$ , restricted by Eq. (26), can be expressed as an integral over  $d\vec{v}'$ , weighted by a density function

$$F(u') = \delta(u' - u - u_0) / \int d\vec{v}'' \delta(u'' - u - u_0).$$

It is easy to show that  $F(u') d\vec{v}' = du' \delta(u' - u - u_0)$ , and therefore the restricted "sum" over velocities  $\vec{v}'$  is equivalent to integration over all energies  $u'$  weighted by the distribution  $\delta(u' - u - u_0)$ . Thus, the collision term can be written

$$\begin{aligned} \Delta \vec{v} \delta f(\vec{v}) / \delta t \Big|_c &= - f(\vec{v}) \Delta \vec{v} v N Q(v) \\ &+ \int du' \delta(u' - u - u_0) f(\vec{v}') \Delta \vec{v}' v' N Q(v'), \end{aligned}$$

where the first term represents scattering out of (and the second term scattering into) the region  $[\vec{v}, \vec{v} + \Delta \vec{v}]$  of velocity space. From Eq. (27) it follows that the collision term can be expressed as

$$\left. \delta f(\vec{v}) / \delta t \right|_c = (N/v) \left[ f(\vec{v}') v'^2 Q(v') \right]_{v'^2 = v^2 + 2eu_0/m} - f(\vec{v}) v^2 Q(v) \quad (28)$$

To lowest order in the expansion (20),  $f(\vec{v}) = f_0(v)$  depends only upon the magnitude  $v$ , as is the case for  $Q(v)$ , and therefore all quantities can be expressed as functions of the energy  $u$ . Thus, the lowest order inelastic collision term becomes

$$\left. \delta f_0(u) / \delta t \right|_c^{\text{in}} = \frac{2e}{mv} N \left[ (u+u_0) f_0(u+u_0) Q(u+u_0) - u f_0(u) Q(u) \right], \quad (29)$$

where Eq. (24) and (28) have been used. For all collision processes (both elastic and inelastic), there will be a contribution to  $\delta f_0 / \delta t|_c$  originating from momentum transfer. (Whenever an electron of energy  $u$  undergoes a collision process with a neutral molecule of mass  $M$ , there is a transfer of energy of order  $\sim (m/M)u$  resulting from momentum conservation.) The momentum transfer contribution is <sup>7-10</sup>:

$$\left. \delta f_0(u) / \delta t \right|_c^{\text{el}} = \frac{2e}{mv} (d/du) \left[ u^2 \sum_X \frac{2m}{M_X} N_X Q_X^X(u) \left( f_0 + \frac{kT}{e} \frac{df_0}{du} \right) \right] \quad (30)$$

Combining Eq. (25), (29), and (30), we obtain the following form for the Boltzmann equation:

$$\begin{aligned} & (E^2/3) d/du \left[ u df_0/du / \langle NQ_m \rangle \right] + d/du \left[ u^2 \langle (2m/M) NQ_m \rangle \left( f_0 + \frac{kT}{e} \frac{df_0}{du} \right) \right] \\ & + \sum_{\alpha} \left[ (u+u_{\alpha}) f_0(u+u_{\alpha}) N_{\alpha} Q_{\alpha}(u+u_{\alpha}) - u f_0(u) N_{\alpha} Q_{\alpha}(u) \right. \\ & \left. + (u-u_{\alpha}) f_0(u-u_{\alpha}) N_{\alpha}^* Q_{-\alpha}^*(u-u_{\alpha}) - u f_0(u) N_{\alpha}^* Q_{-\alpha}^*(u) \right] = 0 \quad (31) \end{aligned}$$

where  $Q_{\pm\alpha}(u)$  are the (forward and reverse) cross sections for the inelastic collision processes, labeled by  $\alpha$ ,  $N_\alpha$  and  $N_\alpha^*$  are the population densities of the lower and upper (excited) states, and  $u_\alpha$  is the inelastic energy loss associated with the collision. The two weighted averages which occur in Eq. (31) are defined by

$$\langle N Q_m(u) \rangle = \sum_X N_X Q_m^X(u), \quad (32.1)$$

$$\langle (2m/M) N Q_m(u) \rangle = \sum_X (2m/M_X) N_X Q_m^X(u) \quad (32.2)$$

The principle of detailed balance provides relations between the cross sections  $Q_{\pm\alpha}(u)$  for the forward and reverse (superelastic) processes:

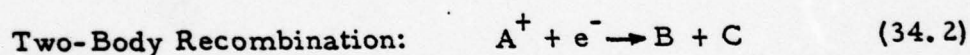
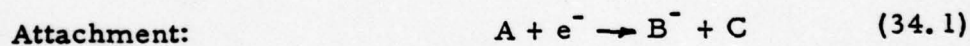
$$(u + u_\alpha) Q_\alpha(u + u_\alpha) = u Q_{-\alpha}(u) \quad (33.1)$$

$$(u - u_\alpha) Q_{-\alpha}(u - u_\alpha) = u Q_\alpha(u) \quad (33.2)$$

The first two terms in the sum over  $\alpha$  in Eq. (31) correspond to collisions in which the electrons lose energy, while the last two terms (which represent the superelastic processes) correspond to collisions in which excited molecular species transfer their energy to the electrons. Only binary electron-molecule collisions, including vibrational excitation, electronic state excitation, attachment, recombination, ionization, etc. will be considered. It should be emphasized, however, that the formulation of the Boltzmann equation as given by Eq. (31) applies only to a quasisteady state situation for which there is no net creation or loss of electrons. If processes such as secondary ionization, electron attachment or recombination are included, Eq. (31) is valid only under condi-



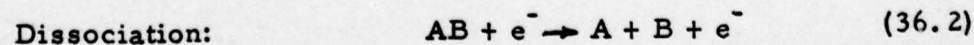
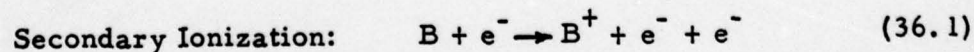
tions for which the collision frequencies for such processes are much lower than those for the inelastic excitation processes which do not involve the creation or loss of electrons. It should be noted that the collision term for such inelastic processes does not contain all four of the terms indicated in the general expression given in Eq. (31). For example, only the second term occurs for recombination or attachment (in which an electron is lost), and for ionization or dissociation, only the first two terms occur (since there is no reverse binary collision process). Because of the low density of states available for momentum conservation, two-body recombination is generally a very slow process. Electron recombination proceeds as a three-body process, which cannot be treated according to the present formulation. However, it is often found experimentally that the rates for three-body recombination vary with pressure as if the process were two-body, and thus, effective cross sections can be used to describe it as a binary collision appropriate for the formulation of Eq. (31). Thus, for (schematic) processes such as



the inelastic collision term in Eq. (31) consists only of

$$- u f_0(u) N_\alpha Q_\alpha(u). \quad (35)$$

For processes such as



the collision term contains only

$$(u+u_{\alpha})f_0(u+u_{\alpha})N_{\alpha}Q_{\alpha}(u+u_{\alpha}) - uf_0(u)N_{\alpha}Q_{\alpha}(u). \quad (37)$$

Furthermore, in the case of secondary ionization, there is the creation of an additional electron. Because experimental knowledge of ionization cross sections is not usually available in the detail necessary to describe the final energy distribution of the created electrons, it is often assumed that the additional electrons are created at zero energy, and that they relax into the distribution on the same time scale (given by the elastic collision frequency) over which the rapid attainment of a quasisteady state occurs. Therefore, the collision term for secondary ionization requires an additional modification, the inclusion of a term

$$\delta(u)N_{\alpha}\int_0^{\infty} du uf_0(u)Q_{\alpha}(u). \quad (38)$$

Perhaps a more realistic hypothesis would be to assume that the final electrons have equal energies or, better still, that their energies are partitioned according to a purely kinematic distribution of a three-body breakup. It is believed that such assumptions, which needlessly complicate the analysis, would provide no additional physical insight. Therefore, the electrons created by secondary ionization are assumed to have zero energy.

The effects of recoil in momentum transfer collisions are included in the second term of Eq. (31), where the molecular energy distribution has been assumed to be Maxwellian at temperature  $T$ . Note that, if there is no electric field and if  $kT$  is much less than the energy thresholds for the inelastic collision processes, then an approximate solution for the electron energy distribution is obtained by equating the

second term of Eq. (31) to zero, giving

$$f_0(u) = \exp [-eu/kT].$$

This is to be expected, since electrons and molecules would be in thermal equilibrium with each other in that case. The momentum transfer term in Eq. (31) is important for low values of  $E/N$  at low temperatures, and for gas mixtures containing light molecules. The physical significance of that term is elastic heating of the molecular gas, to be discussed in more detail in Sec. 2.5. The higher the value of the lowest inelastic excitation threshold, the more important will be the fractional power partition into elastic heating for a given value of  $E/N$ . For molecular gases, characterized by vibrational level excitation processes with very low energy thresholds (typically  $\sim 0.1 - 0.2$  eV), elastic heating is negligible for values of  $E/N$  characteristic of typical laser excitation ( $\geq 3 \times 10^{-17}$  Vcm<sup>2</sup>). However, for rare gas laser mixtures for which the lowest inelastic energy loss usually corresponds to excitation of an electronic level ( $\sim$  few eV), the contribution of elastic heating can be significant even for relatively high values of  $E/N$  (e.g.  $\sim 10^{-16}$  Vcm<sup>2</sup>). Effects of rotational excitation, which are not included in the present version of the electron kinetics analysis, can be incorporated<sup>9, 10</sup> into the Boltzmann equation in the same way as momentum transfer by making a suitable continuum approximation.

Most authors have not only restricted their attention to solution of the Boltzmann equation in the form of Eq. (31), but have often ignored the superelastic collision terms. For weakly excited gases, such an approach is justified, providing that attachment and secondary ionization could be neglected. However, in order to properly describe effects of interest in electrically excited lasers, superelastic collisions must be



included, and in addition, several important extensions to the formulation (31) of the Boltzmann equation are necessary.

First of all, the contribution (38), representing the creation of electrons (at zero energy) from secondary ionization, must be included in the collision term of Eq. (31).

Secondly, it is useful to incorporate a source term  $S_{\text{ext}}(u)$  to describe (as a function of energy) the creation of electrons by external sources of ionization (e.g.,  $e^-$ -beam, photoionization, etc.) and the resulting energy deposition. Since there are often several electron creation processes for which no a priori knowledge of this energy dependence is available (e.g., Penning ionization, photodetachment, photoionization by intracavity radiation), it is convenient to assume that the resulting electron energy is zero. Thus, the source term is assumed to be of the form

$$S_{\text{ext}}(u) = S_0 \delta(u) + S(u), \quad (39)$$

where  $S_0$  represents a rate ( $\text{cm}^{-3} \text{s}^{-1}$ ) of creation of electrons at zero energy, and  $S(u)$  represents a rate of creation per unit energy ( $\text{cm}^{-3} \text{s}^{-1} \text{eV}^{-1}$ ) of electrons of energy  $u$  (i.e.,  $S(u) du$  is the rate of creation of electrons in the energy interval  $[u, u+du]$ ). The first term, which can be used to include all electron creation processes arising from excited-state interactions in the medium, contributes nothing to energy deposition into the electron gas (since the electrons have zero energy). The second term  $S(u)$  is used to describe electron creation from an external source, typically  $e^-$ -beam ionization. A more detailed discussion of energy (power) balance is given in Sec. 2.5.

Third, in order to properly conserve electron number density, a term proportional to  $dn_e/dt$  must be retained from the time-dependent Boltzmann equation. The term  $\partial n_e(u, t)/\partial t$  (where  $n_e(u, t) du = n_e(t) du u^{1/2}$ ,  $f_0(u)$  is the electron density in the energy interval  $[u, u+du]$ ) can be written

$$\begin{aligned} \partial n_e(u, t)/\partial t = & u^{1/2} f_0(u, t) dn_e/dt \\ & + n_e(t) u^{1/2} \partial f_0(u, t)/\partial t. \end{aligned} \quad (40)$$

It is reasonable to retain the earlier assumption that the shape  $f_0(u, t)$  is not an explicit function of the time, since a quasisteady state will be established on a time scale much shorter than that characteristic of molecular and electron kinetic processes. Thus,  $f_0(u)$  will be only an implicit function of time through its dependence upon instantaneous values of various parameters, such as  $E/N$ , and the excited state population densities  $N_\alpha(t)$ . It follows that the second term in Eq. (40) can be deleted, and the explicit time dependence in  $f_0(u, t)$  suppressed in the first term. The first term must be retained, even in the quasisteady state approximation, since it represents the net rate of creation (or loss) of electrons on the time scale of attachment, recombination, ionization, etc. It will be shown that retention of the  $dn_e/dt$  term is necessary to insure that the first integral of the Boltzmann equation correctly results in the conservation equation for the electron number density  $n_e(t)$ . Since  $dn_e/dt$  occurs as a parameter whose value cannot be determined until the equation is solved, a self-consistent iterative method (to be discussed in more detail later) was developed.

Finally, the effects of Coulomb scattering can become important<sup>15, 21</sup>

under conditions of high fractional ionization, so electron-electron collisions must be included. (Charged particle interactions between electrons and heavy ions will be neglected in the present analysis.) For a highly ionized gas, electron-electron collisions dominate electron-molecule collisions, and this tends to force the electron energy distribution to become more nearly Maxwellian. Rockwood<sup>15</sup> has shown how the Boltzmann equation can be expressed in terms of a "flux divergent" description of the electron distribution in energy space, and how electron-electron collisions can be incorporated into such a formulation.

Accounting for these refinements, the Boltzmann equation becomes

$$\begin{aligned}
 u^{1/2} f_0(u) \frac{dn_e}{dt} + \frac{dJ_f(u)}{du} + \frac{dJ_{e1}(u)}{du} + \frac{dJ_{ee}(u)}{du} = \\
 S_0 \delta(u) + S(u) + n_e \sqrt{\frac{2e}{m}} \left\{ \delta(u) \sum_i N_i \int_0^\infty du u f_0(u) Q_i(u) + \right. \\
 \sum_\alpha \left[ (u+u_\alpha) f_0(u+u_\alpha) N_\alpha Q_\alpha(u+u_\alpha) - u f_0(u) N_\alpha Q_\alpha(u) \right. \\
 \left. \left. + (u-u_\alpha) f_0(u-u_\alpha) N_\alpha^* Q_{-\alpha}(u-u_\alpha) - u f_0(u) N_\alpha^* Q_{-\alpha}(u) \right] \right\}. \quad (41)
 \end{aligned}$$

The sum over  $i$  represents a sum over all secondary ionization processes. The sum over  $\alpha$  corresponds to the complete set of all inelastic electron-molecule collisions, including ionization, with the tacit understanding (according to the foregoing discussion) that certain terms in the general collision expression are to be omitted for processes for which there is a net creation or loss of electrons, or for which there is no reverse binary collision. (I. e., the collision term is reduced to the expressions (35) or (37) in such cases.) The "current densities"  $J_f(u)$ ,



$J_{el}(u)$ , and  $J_{ee}(u)$ , which correspond to a flux of electrons in energy space driven by the applied electric field, elastic scattering collisions, and electron-electron collisions, are defined by

$$J_f(u) = - (E^2/3) n_e \sqrt{\frac{2e}{m}} \left[ u \frac{df_0}{du} / \langle N Q_m(u) \rangle \right] \quad (42.1)$$

$$J_{el}(u) = - n_e \sqrt{\frac{2e}{m}} u^2 \langle (2m/M) N Q_m(u) \rangle \left[ f_0 + \frac{kT}{e} \frac{df_0}{du} \right] \quad (42.2)$$

$$J_{ee}(u) = - (2\pi/3) n_e^2 \sqrt{\frac{2e}{m}} (q^4/e^2) \ln \Lambda \left[ P(u) \frac{df_0}{du} + Q(u) f_0 \right] \quad (42.3)$$

where

$$P(u) = 2 \int_0^u dw w^{3/2} f_0(w) + 2u^{3/2} \int_u^\infty dw f_0(w), \quad (43.1)$$

$$Q(u) = 3 \int_0^u dw w^{1/2} f_0(w). \quad (43.2)$$

In the above equations,  $q = 300e = 4.8 \times 10^{-10}$  esu is the electronic charge (cgs units),  $e = 1.602 \times 10^{-12}$  erg/eV, and  $\Lambda$  is the ratio of the Debye length  $\ell_D$  and the classical distance of closest approach  $r_0$  (for an electron of average energy  $u = \bar{u}$ ), defined by

$$\Lambda = \ell_D / r_0 \quad (44)$$

$$\ell_D = (kT_e / 4\pi n_e^2)^{1/2} \quad (45)$$

$$r_0 = q^2 / (e\bar{u}) = 2q^2 / 3kT_e. \quad (46)$$

Comparison of Eq. (31) with Eq. (41) shows that they are equivalent, except for the inclusion of the additional terms  $dn_e/dt$  for electron conservation,  $S(u)$  for external ionization sources,  $dJ_{ee}(u)/du$  for electron-electron collisions, and the term  $\sim\delta(u)$  representing the creation of electrons (at zero energy) by secondary ionization and the external source  $S_0$ . The formulation (41) of the Boltzmann equation to be used in the present analysis is written in such a way that its significance as a continuity equation (in energy space) is manifestly apparent. In Fig. 2.6, an interval  $[u, u + du]$  of energy space is depicted, with an electron "current density"  $J(u)$ . If there is an external source  $S_{ext}(u)$  and a (non-local) source  $S_{coll}(u)$  from inelastic collisions driving electrons into (and out of) the interval  $[u, u + du]$ , the continuity equation can be written

$$du[dn_e(u, t)/dt] + [J(u+du) - J(u)] = du[S_{ext}(u) + S_{coll}(u)]$$

or,

$$dn_e(u, t)/dt + dJ(u)/du = S_{tot}(u) \quad (47)$$

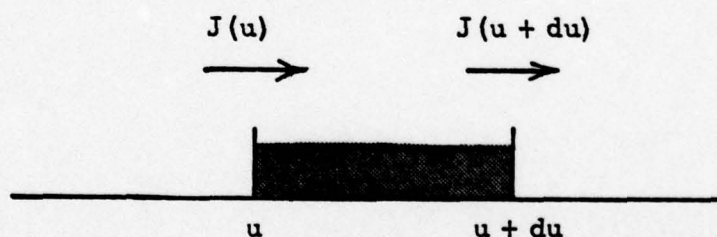


Fig. 2.6: Continuity equation interval.

Thus, the first term on the left hand side of Eq. (41) represents the rate of change of electron density in the interval  $[u, u + du]$ , while the  $dJ/du$  terms represent electron flux in energy space driven by the applied electric field, elastic collisions, and electron-electron scattering. On the right hand side of (41), there are source terms from ex-

ternal ionization, secondary ionization, and nonlocal inelastic scattering of electrons into and out of the interval  $[u, u+du]$ .

The normalization condition for  $f_0(u)$  is taken to be

$$\int_0^{\infty} du u^{1/2} f_0(u) = 1, \quad (48)$$

where the factor  $u^{1/2}$  originates from the density of states associated with the transformation from the three-dimensional velocity space  $\vec{v}$  to the energy space  $u$ :  $d\vec{v} = 4\pi v^2 dv = 2\pi(2e/m)^{3/2} u^{1/2} du$ . (Thus, the units of  $f_0(u)$  will be  $eV^{-3/2}$ .) From the solution  $f_0(u)$  of the Boltzmann equation (41), all of the forward and reverse electron excitation rates  $\langle v Q_{\pm\alpha}(u) \rangle$ , electrical power partitioning, and miscellaneous plasma parameters (drift velocity  $v_d$ , mobility  $\mu$ , average and characteristic energies  $\bar{u}$  and  $\epsilon_k$ , effective temperature  $T_e$ , etc.) can be obtained:

Collision Rates ( $cm^3/s$ ):

$$\langle v Q_{\pm\alpha}(u) \rangle = (2e/m)^{1/2} \int_0^{\infty} du u f_0(u) Q_{\pm\alpha}(u) \quad (49)$$

Mobility ( $cm^2/Vs$ ):

$$\mu = -(1/3)(2e/m)^{1/2} \int_0^{\infty} du [u / \langle N Q_m(u) \rangle] df_0/du \quad (50)$$

Diffusion Coefficient ( $cm^2/s$ ):

$$D = (1/3)(2e/m)^{1/2} \int_0^{\infty} du [u / \langle N Q_m(u) \rangle] f_0(u) \quad (51)$$

Average Energy (eV):

$$\bar{u} = \int_0^{\infty} du u^{3/2} f_0(u) \quad (52)$$



Effective Temperature (K):

$$T_e = (2/3) \bar{u}/k \quad (53)$$

Characteristic Energy (eV):

$$\epsilon_k = D/\mu \quad (54)$$

Drift Velocity (cm/s):

$$v_d = \mu E \quad (55)$$

For the case of an ac electric and/or applied magnetic fields, there are other transport coefficients of interest, and expressions for these quantities as well as discussion of the extensions of the Boltzmann equation required to describe these phenomena can be found in the references<sup>8-10</sup>.

The first integral (from 0 to  $\infty$ ) of Eq. (41) gives an expression for the conservation of electron density:

$$dn_e/dt = n_e[\nu_i - \nu_a] + \int_0^\infty du S(u) + S_0, \quad (56)$$

where

$$\nu_i = \sum_i N_i \langle v Q_i(u) \rangle \quad (57)$$

and

$$\nu_a = \sum_a N_a \langle v Q_a(u) \rangle \quad (58)$$

are the total secondary ionization and electron attachment frequencies. Note that for all of the inelastic scattering processes which conserve

electrons, the integral over the collision term vanishes:

$$\int_0^{\infty} du \left[ (u+u_{\alpha}) f_0(u+u_{\alpha}) Q_{\alpha}(u+u_{\alpha}) - u f_0(u) Q_{\alpha}(u) \right] = 0, \quad (59)$$

which can be shown by shifting the variable of integration and noting that  $Q_{\alpha}(u) = 0$  for  $u < u_{\alpha}$ . For attachment or recombination, however, only the term (35) occurs in the collision expression, leaving the  $\nu_a$  term in Eq. (56). For secondary ionization, both terms shown in Eq. (59) appear and the integral vanishes; however, there is still a term in Eq. (56) containing  $\nu_i$  originating from the  $\delta(u)$  term in Eq. (41). The integral of  $S(u)$  on the right hand side represents the total rate of change of electron density from the external source.

It is apparent that the term proportional to  $dn_e/dt$  must be retained in order to correctly obtain conservation of electron density in situations where creation or loss of electrons is important. Obviously, this will always be the case for transient analysis of pulsed electrical lasers if it is important to properly describe the build-up of the plasma. Note that Eq. (31), which does not include the  $dn_e/dt$  term, may give rise to solutions for  $f_0(u)$  which contain logarithmic singularities at  $u = 0$ . To demonstrate this, consider the case of attachment only, and integrate the Boltzmann equation from  $u$  to  $\infty$ :

$$J(\infty) - J(u) = -n_e \nu_a$$

As  $u \rightarrow 0$ , (since  $J(\infty) = 0$ ), this becomes an equation of the form

$$[Au^2 + Bu] df_0/du = n_e \nu_a$$

which is characterized by a singularity at  $u = 0$ .

If Eq. (41) is multiplied by  $eu$  and integrated over all energy, an expression for electrical power balance is obtained:

$$\begin{aligned}
e n_e \mu E^2 + \int_0^{\infty} du (eu) S(u) &= e \bar{u} dn_e/dt + \\
n_e e (2e/m)^{1/2} \left\{ \int_0^{\infty} du u^2 \langle (2m/M) N Q_m \rangle \left[ f_0 + (kT/e) df_0/du \right] \right. \\
&\left. + \sum_{\alpha} u_{\alpha} \int_0^{\infty} du u f_0(u) \left[ N_{\alpha} Q_{\alpha}(u) - N_{\alpha}^* Q_{-\alpha}(u) \right] \right\} \quad (60)
\end{aligned}$$

The form of the inelastic collision term on the RHS of Eq. (60) results from a change of variables in the first term of an expression, such as

$$\begin{aligned}
N_{\alpha} \left\{ \int_0^{\infty} du u (u + u_{\alpha}) f_0(u + u_{\alpha}) Q_{\alpha}(u + u_{\alpha}) - \int_0^{\infty} du u^2 f_0(u) Q_{\alpha}(u) \right\} \\
= N_{\alpha} \int_0^{\infty} du f_0(u) Q_{\alpha}(u) [u(u - u_{\alpha}) - u^2] \\
= -N_{\alpha} u_{\alpha} \int_0^{\infty} du u f_0(u) Q_{\alpha}(u) \quad (61)
\end{aligned}$$

Note that, for processes such as ("two-body") electron recombination and attachment (in which an electron is lost), only the second term of the form (35) (i.e.,  $-u f_0(u) N_{\alpha} Q_{\alpha}(u)$ ) occurs in Eq. (41). In that case, the first term on the LHS of Eq. (61) is absent and the corresponding term in the power balance equation (60) must be modified:

$$N_{\alpha} \int_0^{\infty} du u^2 f_0(u) Q_{\alpha}(u) \quad (62)$$

The physical interpretation of Eq. (60) is that the total electrical input power density (discharge and external deposition) on the left hand side is partitioned into  $e \bar{u} dn_e/dt$  (representing the rate of change of electron



kinetic energy stored in the electron gas), elastic heating from momentum transfer collisions, and dissipation by the inelastic excitation processes on the right hand side. Note that the contribution from electron-electron scattering vanishes--this mechanism merely redistributes the electron energy and tends to drive the distribution toward a Maxwellian shape. To show that the electron-electron contribution vanishes, integrate by parts,

$$\int_0^{\infty} du u dJ_{ee}(u)/du = J_{ee}(u) \Big|_0^{\infty} - \int_0^{\infty} du J_{ee}(u), \quad (63)$$

and the first term on the right vanishes because  $P(\infty) = 2\bar{u}$ ,  $Q(\infty) = 3$ ,  $P(0) = Q(0) = 0$ , and  $f_0(\infty) = df_0(\infty)/du = 0$ . Thus,

$$\begin{aligned} - \int_0^{\infty} du u dJ_{ee}(u)/du &= \int_0^{\infty} du J_{ee}(u) \\ &= - (2\pi/3) n_e^2 (q^4/e^2) \ln \Lambda \int_0^{\infty} du [P df_0/du + Q f_0(u)] (2e/m)^{1/2} \end{aligned}$$

Suppressing the constant factor, and integrating the first term by parts gives

$$\begin{aligned} \int_0^{\infty} du [P df_0/du + Q f_0] &= P(u) f_0(u) \Big|_0^{\infty} + \int_0^{\infty} du f_0 [Q - dP/du] \\ &= \int_0^{\infty} du f_0(u) [Q(u) - dP/du] \end{aligned} \quad (64)$$

From the definitions (43),

$$Q(u) - dP(u)/du = 3 \left\{ \int_0^u dw w^{1/2} f_0(w) - u^{1/2} \int_u^{\infty} dw f_0(w) \right\} \quad (65)$$

and the expression in (64) becomes

$$\int_0^{\infty} du f_0(u) [Q(u) - dP(u)/du] =$$

$$3 \left\{ \int_0^{\infty} du f_0(u) \int_0^u dw w^{1/2} f_0(w) - \int_0^{\infty} du u^{1/2} f_0(u) \int_u^{\infty} dw f_0(w) \right\}$$

Interchanging the variables (u, w) in the second term above gives

$$\int_0^{\infty} du f_0(u) [Q(u) - dP(u)/du] =$$

$$3 \left\{ \int_0^{\infty} \int_0^u - \int_0^{\infty} \int_w^{\infty} \right\} du dw w^{1/2} f_0(u) f_0(w) = 0 \quad (66)$$

Since both of the integrals in Eq. (66) are carried out over the same (infinite)  $45^\circ$  sector in the upper half of the (u, w) plane defined by  $0 \leq u < \infty$ ,  $0 \leq w \leq u$ , the electron-electron contribution vanishes.

From the definition of inelastic collision rate given by (49), the power balance equation (60) can be written, finally, as

$$e n_e \mu E^2 + e \langle U^+ \rangle S_b = e \bar{u} dn_e/dt +$$

$$e n_e (2e/m)^{1/2} \int_0^{\infty} du u^2 \langle (2m/M) N Q_m \rangle \left[ f_0 + (kT/e) df_0/du \right]$$

$$+ n_e \sum_{\alpha} (eu_{\alpha}) \left[ N_{\alpha} \langle v Q_{\alpha}(u) \rangle - N_{\alpha}^* \langle v Q_{-\alpha}(u) \rangle \right]$$

$$+ n_e e (2e/m)^{1/2} \sum_a N_a \int_0^{\infty} du u^2 f_0(u) Q_a(u) \quad (67)$$

where the sum over "a" is over all attachment and recombination pro-

cesses, which are to be implicitly excluded from the sum over all the other inelastic collisions  $\alpha$ .  $S_b$  is the total rate of creation of electrons with positive energies,

$$S_b = \int_0^{\infty} du S(u) \quad (68)$$

and an average deposition energy  $\langle U^+ \rangle$  has been defined as a weighted average of the external ionization source function  $S(u)$  as

$$\langle U^+ \rangle = \int_0^{\infty} du u S(u) / \int_0^{\infty} du S(u). \quad (69)$$

The typical source of external ionization is a high energy electron beam. The mathematical description of the energy deposition in the gas is, in general, quite complicated and several investigators have developed extensive computer programs for such analysis. It is beyond the scope of the present work to describe the physics of  $e^-$ -beam ionization, so it is not possible to indicate how the form of the excitation source function  $S(u)$  is determined. If the origin of the source ionization is an external  $e^-$ -beam of current density  $J_b$  ( $A/cm^2$ ), then the function  $S(u)$  could be expressed in terms of cross sections  $\sigma_i^+(u)$  as

$$S(u) = (J_b/e) \sum_i \sigma_i^+(u) N_i, \quad (70)$$

where the sum is over all species  $i$  ionized by the beam. The total deposition of  $e^-$ -beam energy associated with ionization is then

$$e \langle U^+ \rangle S_b = \langle U^+ \rangle \sum_i \sigma_i^+ N_i J_b = J_b dV^+/dx, \quad (71)$$



where  $\sigma_i^+ = \int du \sigma_i^+(u)$ , and an effective voltage drop has been defined as  $dV^+/dx = \langle U^+ \rangle / \ell$  in terms of a "mean free path"  $\ell$  for ionization,

$$\ell^{-1} = \sum_i \sigma_i^+ N_i. \quad (72)$$

A similar term  $dV^*/dx$  occurs for  $e^-$ -beam deposition corresponding to excited states.

### Numerical Approach

The numerical solution of the Boltzmann equation (41) is carried out by reducing the differential equation to a finite difference equation, defined over a uniform grid of equally spaced energy values ( $0 = u_1, u_2, u_3, \dots, \dots, u_M = u_{\max}$ ), where the maximum energy  $u_{\max}$  satisfies, typically,  $u_{\max} \geq 5\bar{u}$ . This results in a large set of coupled algebraic equations (typically  $M > 500$ ) which could be solved (at least formally) by a matrix inversion. However, a straightforward matrix inversion is not practical computationally or from the standpoint of computer core storage that would be required. For example, a typical energy range of (0, 20) eV, subdivided into a mesh of  $M = 500$  to give an energy resolution of 0.04 eV, would require storage and manipulation of  $500 \times 500$  matrices, each of which would contain  $250,000 \approx 1,000,000$  elements. To reduce the problem of core storage and matrix inversion, an iterative approach that utilizes the advantages of sparse matrices (i.e. matrices whose elements are mostly zeros) has been developed. The essence of the present technique<sup>16</sup> is the reduction of the system of linear difference equations to a form which involves the inversion of only tridiagonal matrices, for which computation time and core storage are substantially reduced.

With some recent exceptions, most of the work which has been done to

implement the numerical solution of the Boltzmann equation has been associated with problems for which the excited state population densities are negligible, and for which the superelastic collision terms can therefore be omitted. In that case, electrons always lose energy in collisions, and for any given energy  $u$  the inelastic collision term on the right hand side of (41) involves only  $f_0(u)$  and  $f_0(u + u_\alpha)$ --i.e. the values for the distribution function  $f_0$  evaluated at energies equal to and greater than  $u$ . Therefore, one of the most common approaches to the numerical solution of the Boltzmann equation has been to assume a fixed value for  $f_0(u_{\max})$ , integrate (41) backward from  $u = u_{\max}$  to  $u = 0$ , and finally to impose the normalization condition (48). If the superelastic terms are retained, then terms containing  $f_0(u - u_\alpha)$  occur, and the backward integration scheme fails. Attempts to extend this technique to the superelastic case have generally encountered difficulties and limited success.

Under highly excited conditions typical of laser plasmas ( $N^*/N \gtrsim 10^{-5}$ ), superelastic collision terms must be retained. Their inclusion presents no difficulties for the present technique, which is based upon an iterative solution of the set of linear difference equations obtained from (41) and reduced to tridiagonal form. The algorithm developed is extremely fast, and execution speed is optimized when a good initial guess for  $f_0$  is available. Thus, the present approach is especially suitable for a coupled analysis in which the excited state population densities and discharge voltage change as a function of time, since the previous electron distribution (at some time  $t$ ) provides a good initial guess for obtaining the updated distribution (at time  $t + \Delta t$ ). As an example: for an electron grid of 500 points, with 15 inelastic collision processes and electron-electron scattering, the electron distribution function  $f_0$  converged to an accuracy  $< 2 \times 10^{-3}$  after  $\sim 8$  iterations in  $\sim 0.7$  CF sec-

onds on the CDC 6600 computer (from an initial guess for  $f_0(u)$  given by  $e^{-eu/kT}$ , for example). The numerical techniques for the solution of Eq. (41) will be described in detail below.

The functional values of the distribution  $f_0(u)$  defined over the uniform grid of energy values ( $0 = u_1, u_2, u_3, \dots, u_M = u_{\max}$ ) shown in Fig. 2.7 will be denoted by  $(f_1, f_2, f_3, \dots, f_M)$ , and the spacing of the energy grid will be denoted by  $\Delta u$ :

$$\begin{aligned} M &= \text{MESH} + 1 \\ \Delta u &= u_{\max} / \text{MESH} \\ u_i &= (i - 1) \Delta u \\ f_i &= f_0(u_i) \end{aligned} \tag{73}$$

where  $i = 1, 2, 3, \dots, M$ .

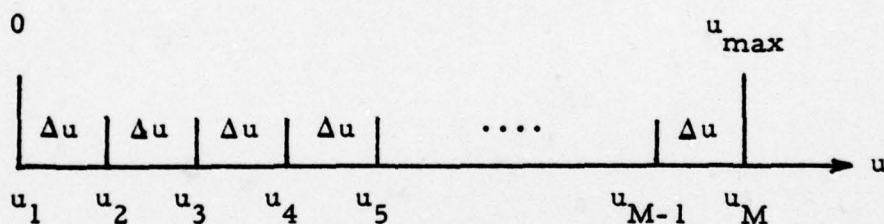


Fig. 2.7: Uniform energy grid.

If Eq. (41) is integrated from  $(u_i - \Delta u/2)$  to  $(u_i + \Delta u/2)$  for  $i = 2, 3, 4, \dots, M$ , with the tacit boundary condition that  $f_{M+1} = 0$ , the result is a system of  $(M - 1)$  coupled algebraic equations:



$$\begin{aligned}
& \left\{ J_f(u) + J_{el}(u) + J_{ee}(u) \right\} \bigg|_{u_i - \Delta u/2}^{u_i + \Delta u/2} + \frac{dn_e}{dt} \int_{u_i - \Delta u/2}^{u_i + \Delta u/2} du u^{1/2} f_0(u) = \\
& \int_{u_i - \Delta u/2}^{u_i + \Delta u/2} du \left[ S(u) + (n_e \nu_i + S_0) \delta(u) \right] + \\
& n_e \sqrt{\frac{2e}{m}} \sum_{\alpha} \int_{u_i - \Delta u/2}^{u_i + \Delta u/2} du \left[ (u + u_{\alpha}) f_0(u + u_{\alpha}) N_{\alpha} Q_{\alpha}(u + u_{\alpha}) - u f_0(u) N_{\alpha} Q_{\alpha}(u) \right. \\
& \left. + (u - u_{\alpha}) f_0(u - u_{\alpha}) N_{\alpha}^* Q_{-\alpha}(u - u_{\alpha}) - u f_0(u) N_{\alpha}^* Q_{-\alpha}(u) \right] \quad (74)
\end{aligned}$$

All of the integrals which occur in Eq. (74) will be approximated by the values of the integrand taken at the midpoint  $u_i$ . The values of  $f_0$  and  $df_0/du$  which occur in Eq. (74) at the midpoint energies,

$$u_i^{\pm} = u_i \pm \Delta u/2 \quad (75)$$

are approximated by

$$f_0(u_i \pm \Delta u/2) = f_0(u_i^{\pm}) = (f_{i\pm 1} + f_i)/2 \quad (76.1)$$

$$f_0'(u_i \pm \Delta u/2) = f_0'(u_i^{\pm}) = \pm (f_{i\pm 1} - f_i)/\Delta u. \quad (76.2)$$

For convenience, we define the following functions:

$$\begin{aligned}
p(u) = & (E^2/3) u / \langle N Q_m(u) \rangle + (kT/e) u^2 \langle (2m/M) N Q_m(u) \rangle \\
& + (2\pi/3) (q^4/e^2) n_e \ln \Lambda P(u) \quad (77)
\end{aligned}$$

$$q(u) = u^2 \langle (2m/M) N Q_m(u) \rangle + (2\pi/3) (q^4/e^2) n_e \ln \Lambda Q(u) \quad (78)$$

in terms of which the total "current density" can be expressed as

$$\begin{aligned} J(u) &= J_f(u) + J_{el}(u) + J_{ee}(u) \\ &= -n_e (2e/m)^{1/2} \left[ p(u) \frac{df_0}{du} + q(u) f_0(u) \right] \end{aligned} \quad (79)$$

With the above definitions and approximations, Eq. (74) becomes

$$\begin{aligned} &- p(u_i^+) (f_{i+1} - f_i) / \Delta u + p(u_i^-) (f_i - f_{i-1}) / \Delta u - q(u_i^+) (f_{i+1} + f_i) / 2 \\ &+ q(u_i^-) (f_i + f_{i-1}) / 2 + (2e/m)^{-1/2} \Delta u \left[ \frac{n_e}{n_e} u_i^{1/2} f_i - \frac{S_i}{n_e} - \delta_{i,2} \left( \nu_i + \frac{S_0}{n_e} \right) / \Delta u \right] \\ &= \Delta u \sum_{\alpha} \left[ (u_i + u_{\alpha}) f_0(u_i + u_{\alpha}) N_{\alpha} Q_{\alpha}(u_i + u_{\alpha}) - u_i f_i N_{\alpha} Q_{\alpha}(u_i) \right. \\ &\quad \left. + (u_i - u_{\alpha}) f_0(u_i - u_{\alpha}) N_{\alpha}^* Q_{-\alpha}(u_i - u_{\alpha}) - u_i f_i N_{\alpha}^* Q_{-\alpha}(u_i) \right] \end{aligned} \quad (80)$$

where  $S_i = S(u_i)$ . For convenience, define the quantities

$$\begin{aligned} p_i^{\pm} &= p(u_i^{\pm}) = p(u_i \pm \Delta u / 2) \\ q_i^{\pm} &= q(u_i^{\pm}) = q(u_i \pm \Delta u / 2) \end{aligned} \quad (81)$$

The  $\delta$ -function in Eq. (41) and (74) is approximated by a rectangular spike of thickness  $\Delta u$  and amplitude  $1/\Delta u$ . Separate the collision term in Eq. (80) into "diagonal" (i.e., containing  $f_0(u_i) = f_i$ ) and "off-diagonal" elements (i.e. containing  $f_0(u_i \pm u_{\alpha})$ ) and use the detail balance relations (33) to define

$$D_i = \sum_{\alpha} \left[ u_i N_{\alpha} Q_{\alpha}(u_i) + (u_i + u_{\alpha}) N_{\alpha}^* Q_{\alpha}(u_i + u_{\alpha}) \right] \quad (82)$$

and

$$T_i = \sum_{\alpha} \left[ (u_i + u_{\alpha}) f_o(u_i + u_{\alpha}) N_{\alpha} Q_{\alpha}(u_i + u_{\alpha}) + u_i f_o(u_i - u_{\alpha}) N_{\alpha}^* Q_{\alpha}(u_i) \right] \quad (83)$$

Eq. (80) can be rearranged to give

$$a_{i,i-1} f_{i-1} + a_{i,i} f_i + a_{i,i+1} f_{i+1} = b_i, \quad (84)$$

$i = 2, 3, \dots, M$ , to form a system of  $(M-1)$  equations for  $M$  unknowns  $(f_1, f_2, f_3, \dots, f_M)$ , with coefficients defined by

$$\begin{aligned} a_{i,i-1} &= p_i^- / \Delta u - q_i^- / 2 \\ a_{i,i+1} &= p_i^+ / \Delta u + q_i^+ / 2 \\ a_{i,i} &= - (p_i^+ + p_i^-) / \Delta u + (q_i^+ - q_i^-) / 2 \\ &\quad - \Delta u \left[ u_i^{1/2} (2e/m)^{-1/2} \dot{n}_e / n_e + D_i \right] \\ b_i &= - \Delta u \left[ T_i + (2e/m)^{-1/2} [S_i / n_e + \delta_{i,2} (\nu_i + S_o / n_e) / \Delta u] \right], \end{aligned} \quad (85)$$

for  $i = 2, 3, \dots, M$ . Note that the diagonal terms have been placed on the LHS, and the off-diagonal terms on the RHS of Eq. (84). There is, obviously, considerable latitude in the definition of coefficients (e.g., Eq. (85)) for the reduction of the Boltzmann equation to the form (84). The essential criterion is that any such choice be suitable for numerical implementation by a convergent and computationally efficient algorithm for solution.



The set of  $(M - 1)$  equations (84) can be completed with an  $M$ th equation in a variety of ways. The simplest approximation, which has been found to be quite satisfactory, is to take  $f_1 = f_2$ . After the iterative calculation of  $f$  converges, the magnitude is adjusted to satisfy the required normalization condition (48). Thus, Eq. (85) is supplemented by

$$a_{1,1} = b_1 = 0; \quad a_{1,0} = a_{1,2} = 0 \quad (86)$$

and the complete set of  $M$  equations in  $M$  unknowns can be written

$$\begin{aligned} a_{1,1} f_1 &= b_1 \\ a_{2,1} f_1 + a_{2,2} f_2 + a_{2,3} f_3 &= b_2 \\ a_{3,2} f_2 + a_{3,3} f_3 + a_{3,4} f_4 &= b_3 \\ &\vdots \\ &\vdots \\ &\vdots \\ &\vdots \\ a_{M,M-1} f_{M-1} + a_{M,M} f_M &= b_M \end{aligned} \quad (87)$$

in which form they resemble a linear tridiagonal system. It should be kept in mind, however, that they are neither linear or tridiagonal; the electron-electron scattering contribution makes  $p(u)$  and  $q(u)$  (and therefore, the coefficients  $a_{i,i}$ ,  $a_{i,i \pm 1}$ ) dependent upon  $f_0(u)$ , and the vector  $b_i$  contains off-diagonal elements  $f_0(u_i \pm u_\alpha)$ . Formally, the solution of the finite difference equations could be obtained (in the absence of electron-electron collisions, anyway) by direct matrix inversion, although this is not practical computationally or from the standpoint of computer storage requirements. Instead, the set of equations has been explicitly separated into the form of Eq. (87) in order to implement an iterative

technique which exploits the tridiagonal structure. Eq. (87) can be written in matrix form as

$$A(\vec{f})\vec{f} = \vec{b}(\vec{f}) \quad (88)$$

where

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & & & \\ a_{2,1} & a_{2,2} & a_{2,3} & & \\ & a_{3,2} & a_{3,3} & a_{3,4} & \\ & & \ddots & \ddots & \\ & & & a_{M-1,M} & \\ & & & a_{M,M-1} & a_{M,M} \end{bmatrix} \quad (89)$$

and  $\vec{f} = (f_1, f_2, f_3, \dots, f_M)^T$ ,  $\vec{b} = (b_1, b_2, b_3, \dots, b_M)^T$ . The explicit dependence upon  $\vec{f}$  of the matrix  $A(\vec{f})$  and the vector  $\vec{b}(\vec{f})$  has been expressed in Eq. (77), (78), (81), and (85). To solve the (nonlinear) equation (88), consider a sequence of vectors

$$\{\vec{f}^i\} = \vec{f}^0, \vec{f}^1, \dots, \vec{f}^n, \vec{f}^{n+1}, \dots \quad (90)$$

defined by the iterative equation

$$\begin{aligned} A(\vec{f}^n)\vec{f}^{n+1} &= \vec{b}(\vec{f}^n) \\ \vec{f}^{n+1} &= A(\vec{f}^n)^{-1}\vec{b}(\vec{f}^n), \end{aligned} \quad (91)$$

with the initial vector  $\vec{f}^0$  chosen arbitrarily. If the sequence of vectors  $\{\vec{f}^i\}$  defined by the recursion relation (91) converges, it must necessarily converge to the solution of Eq. (88), independent of the initial

guess chosen for  $\vec{f}^0$ . Since A is tridiagonal, it can be numerically inverted very rapidly by using elementary row manipulations downward (upward) to annihilate the lower (upper) diagonal, followed by back substitution upward (downward). Furthermore, the computer core requirements are substantially reduced, since only three diagonals (rather than a full  $M \times M$  array) of elements need be stored and manipulated.

To implement the iterative technique, an initial guess for  $\vec{f}^0$  is chosen and a sequence  $\{\vec{f}^i\}$  of successively refined approximations is generated using Eq. (91). An acceptable approximation  $\vec{f}^{n+1}$  to the solution of Eq. (88) is assumed to have been attained when the following convergence criterion is satisfied:

$$\text{Max}_i \left| (f_i^{n+1} - f_i^n) / f_i^n \right| < \epsilon \quad (92)$$

The solution  $\vec{f}$  to Eq. (88) is typically exponential, varying over several orders of magnitude in the range  $(0, u_{\max})$ . Therefore, Eq. (92) has been weighted in such a way that the maximum relative (rather than absolute) change in all of the components  $f_i$  of the solution between two successive iterations must be less than  $\epsilon$  for convergence to be declared. Eq. (92) is not rigorous, and probably requires mathematical assumptions about uniform convergence; however, it is physically reasonable and numerically convenient. (To illustrate the need for caution in applying Eq. (92), consider the sequence  $\{S_n\}$  of partial sums,  $S_n = 1 + (1/2) + (1/3) + \dots + (1/n)$ . For any fixed  $\epsilon$  and for  $n$  sufficiently large,  $(S_n - S_{n-1})/S_n = 1/nS_n < \epsilon$ . Although the condition (92) predicts convergence at some point, the sequence  $\{S_n\}$  is known to diverge.)

Note that all of the off-diagonal elements of the inelastic collision term



have been included in the vector  $\vec{b}$ , defined in Eq. (85). Terms involving an energy ( $u_i \pm u_\alpha$ ) are evaluated at the nearest mesh point, or are discarded if the energy lies outside of the range  $[0, u_{\max}]$  chosen for the calculations. (It is important, therefore, to choose a value for  $u_{\max}$  that is suitably large to minimize computational inaccuracies that may result from such numerical "sinks". On the other hand,  $u_{\max}$  cannot be chosen too large without sacrificing energy resolution.)

There are (at least in principle) an infinite number of ways in which Eq. (80) can be represented by a recursive sequence of equations such as (91). There is no a priori guarantee, in general, that an iterative procedure based upon an arbitrary definition of the coefficients for the recursive scheme of Eq. (91) will necessarily converge. In the course of development of the present algorithm, some variations in the definition of the coefficients  $a_{i,j}$  and  $b_i$  were explored. For example, in an attempt to optimize performance, the definition (85) was modified by shifting a fractional part  $\xi$  of some of the diagonal terms in  $a_{i,i}$  to the term  $b_i$  on the RHS of Eq. (84). It was found that, in some cases, the rapidity of convergence could be slightly enhanced by choosing  $\xi > 0$ , although problems were often incurred for large values of  $\xi$  ( $\geq 0.4$ ) for which convergence was sometimes unsuccessful. It has been demonstrated by extensive numerical tests that the system of equations defined by Eq. (85)-(91) do converge (usually), and that they are quite efficient computationally. For the present analysis, therefore, the definition (85) has been adopted for the Boltzmann subroutine.

The coefficient  $a_{i,i}$  defined by Eq. (85) contains the parameter  $\dot{n}_e$ , whose value is not known a priori. The first integral of the Boltzmann equation, Eq. (56), expresses  $\dot{n}_e$  in terms of the secondary ionization, electron attachment and recombination, and external source creation rates. The frequencies  $\nu_i$  and  $\nu_a$  cannot be calculated without knowledge of the elec-

ledge of the distribution function  $f_0(u)$ . Therefore, a self-consistent iterative approach was taken to solve this problem.

An initial estimate (which may be zero) is assumed for  $\dot{n}_e$ , and the Boltzmann equation is solved recursively (as described above) until the convergence criterion of Eq. (92) is satisfied (with an initially coarse choice of  $\epsilon$ , e.g.,  $\epsilon \sim .01$ ). The resulting distribution  $f_0(u)$  is then used to calculate the secondary ionization, attachment, and recombination rates which can be used, along with the external creation rates, to obtain an improved estimate of  $\dot{n}_e$  from Eq. (56). The procedure is repeated until the value for  $\dot{n}_e$  converges to some acceptable accuracy. After convergence relative to the coarse parameter of accuracy is obtained, further refinement can be obtained by making the parameter  $\epsilon$  smaller.

The implementation of these numerical algorithms is accomplished by a FORTRAN subroutine BOLTZ, to be described in more detail in Sec. 3.3 below. In addition, the subroutine is extensively documented with internal COMMENT cards (cf. listing in Vol. II). The present version of Program LASER uses the Boltzmann analysis only for the situation of an electric discharge, although in principle, the formulation should also be applicable to the case of direct  $e^-$ -beam excitation only.



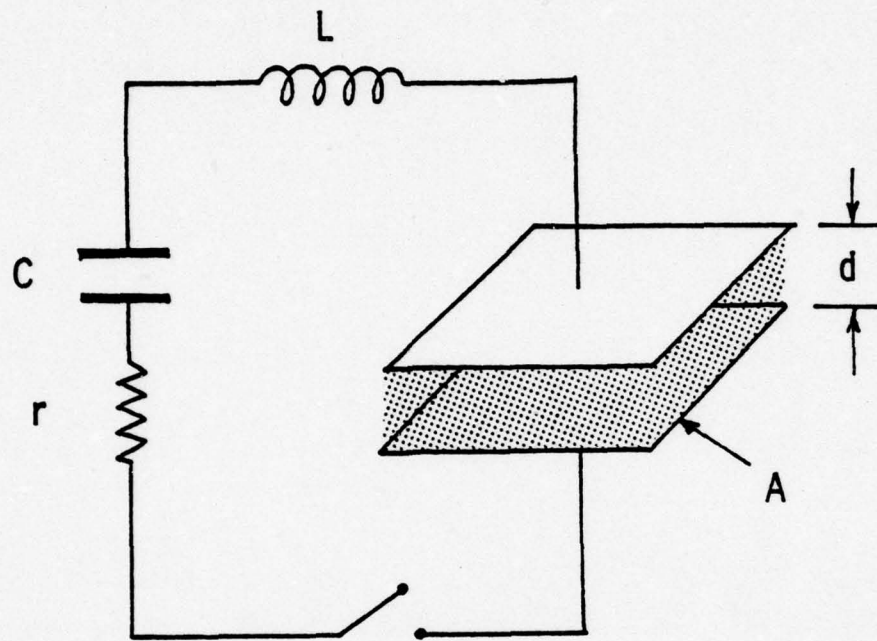
#### 2.4 External Driving Circuit and Ionization Sources

A typical excitation scheme for high power electrical lasers employs a capacitive electric discharge, sustained by an external source of ionization such as a high energy electron beam. In some cases, the additional enhancement of electrical pump power provided by a discharge is not justified in terms of the additional complexity or problems that result, and direct excitation by  $e^-$ -beam alone may be used. The present analysis includes external sources of ionization, as discussed in Sec. 2.3 for the electron kinetics, and couples the kinetic equations to the voltage and current equations for an external driving circuit.

The model for the external driving circuit is shown in Fig. 2.8. A plane parallel discharge of area  $A$ , with anode and cathode separated by a distance  $d$ , is driven by an external RLC circuit with a capacitor initially charged to a high voltage. This discharge is sustained by an external  $e^-$ -beam whose temporal current density  $J_b(t)$  can be specified as an arbitrary function of time. Initially, there is no voltage across the discharge because of the external circuit inductance. As the secondary electron density in the gas changes, the plasma conductivity (and hence the discharge impedance) will change. Thus, the plasma kinetics analysis is directly coupled to the circuit equations which define the instantaneous voltage  $V_d(t)$  (and thus,  $E(t)/N$ ) across the discharge. Although the present model for the external driving circuit is the simplest possible, it nevertheless provides for the description of basic but important phenomena associated with pulsed excitation of the medium. If necessary, more sophisticated circuits (e.g., pulse-forming networks to better match impedance<sup>5</sup>) could be incorporated into the analysis.



# EXTERNAL DRIVING CIRCUIT



Plasma conductivity:  $\sigma = n_e(t)e\mu(t)$

Plasma impedance:  $R_d(t) = d/A\sigma(t)$

$$L \frac{di}{dt} + (r + R_d(t))i + \frac{q}{C} = 0$$

Fig. 2.8: External RLC driving circuit excites gas in a plane-parallel discharge of area A, separation d.

The circuit equations will be formulated as first order differential equations for the charge  $q(t)$  and current  $i(t)$  in order to incorporate them on an equal basis with the molecular kinetic equations (4), the full set of which are integrated numerically using the Gear<sup>6</sup> technique. Thus,

$$dq/dt = i(t) \quad (93.1)$$

$$L di/dt = -q/C - (r + R_d(t)) i \quad (93.2)$$

where  $L$  = inductance,  $r$  = external resistance, and  $C$  = capacitance. If the case  $L = 0$  is desired, only one circuit equation is required:

$$dq/dt = q/(r + R_d(t)) C \quad (94)$$

The discharge impedance  $R_d(t)$  is a function of time, given by

$$R_d(t) = d/A\sigma(t), \quad (95)$$

where

$$\sigma(t) = n_e(t) e \mu(t) \quad (96)$$

is the plasma conductivity as a function of the instantaneous electron density  $n_e(t)$  and the mobility  $\mu(t)$ . The voltage across the discharge,

$$V_d(t) = i(t) R_d(t) \quad (97)$$

determines the value of

$$E(t)/N = V_d(t)/dN \quad (98)$$

If Eq. (93.2) is multiplied by  $i(t)$ , an expression for the conservation of energy (power) is obtained:

$$d/dt (Li^2/2) + i^2 r + (Ad) \sigma E^2 = -d/dt (q^2/2C). \quad (99)$$

The physical interpretation of Eq. (99) is that the rate of change of stored inductive energy ( $Li^2/2$ ), plus power dissipated in the external resistor ( $i^2 r$ ) and deposited into the discharge, is equal to the rate of change of stored energy in the capacitor ( $q^2/2C$ ). The discharge power density

$$\sigma E^2 = n_e(t) e \mu(t) E^2 \quad (100)$$

has occurred previously in Eq. (67) for electrical power partitioning. In the following section, the overall power balance equation for the complete coupled system will be discussed.

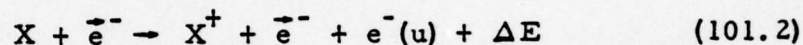
## 2.5 Conservation of Energy

In the foregoing sections, 2.1 - 2.4, equations for power balance have been developed for each component of the coupled analysis. It is now appropriate to combine these results and to formulate a power balance relation for the complete system. The physical interpretation of the parameter  $\Delta E(\alpha)$  for each reaction determines its physical significance in the power balance equation. To begin, therefore, some further discussion devoted to interpretation of the terms of Eq. (5) for specific types of kinetic reactions is required. This will provide the opportunity to describe the typical types of reactions permitted, and various conventions or restrictions on syntax.



### Electron-Beam Collisions

It is beyond the scope of the present analysis to give a rigorous treatment of electron-beam energy deposition in a gas, although provisions have been made for the inclusion of high-energy electron collision processes in the molecular kinetic reaction scheme in terms of a simple rate constant formulation. Excitation and ionization of the molecular species  $X$  by collision with high-energy electrons  $\bar{e}^-$ ,



are described in terms of cross sections  $\sigma^*$  and  $\sigma^+(u)$ , respectively. It is assumed that the medium is isotropically excited and "thin", so that the approximation of single scattering may be made. Adjustments for the effects of multiple scattering can be made in a qualitative way by multiplying the cross sections by an effective scale factor if some a priori knowledge of electron-beam deposition as a function of electron energy, gas mixture, and gas pressure is available. In terms of the  $e^-$ -beam current density  $J_b$  ( $A/cm^2$ ), the rates for reactions (101) are

$$-d[X]/dt = d[X^*]/dt = (J_b \sigma^*/e)[X] \quad (102.1)$$

$$-d[X]/dt = d[X^+]/dt = (J_b \sigma^+/e)[X] \quad (102.2)$$

where  $\sigma^+ = \int du \sigma^+(u)$ . The energies  $\Delta E$ , as defined by Eq. (6), for the two reactions (101) are  $\Delta E = -eu^*$  and  $\Delta E = -eu^+$  respectively, where  $u^*$  and  $u^+$  are excitation and ionization energies (eV). Thus, the contribution of  $e^-$ -beam collisional excitation to the molecular power

balance Eq. (5) becomes

$$\sum_i (eu_i^*) d[X_i^*]/dt = J_b \sum_i u_i^* \sigma_i^*[X_i] \quad (103.1)$$

$$\sum_i (eu_i^+) d[X_i^+]/dt = J_b \sum_i u_i^+ \sigma_i^+[X_i] \quad (103.2)$$

where the sums are over all species which are excited or ionized by the  $e^-$ -beam. Strictly speaking, the reverse process for reaction (101.1) should also be included, although its contribution can usually be neglected in Eq. (103.1). When Eq. (67) for electron power balance is added to Eq. (5) for the molecular power balance, it is apparent that the contribution of the  $e^-$ -beam will be given by

$$\begin{aligned} J_b dV/dx &= J_b \sum_i \left[ u_i^* \sigma_i^* + u_i^+ \sigma_i^+ + \int_0^\infty du u \sigma_i^+(u) \right] [X_i] \\ &= J_b \sum_i \left[ u_i^* \sigma_i^* + \left\{ u_i^+ + \langle U^+ \rangle \right\} \sigma_i^+ \right] [X_i], \end{aligned} \quad (104)$$

where  $dV/dx$  is an effective voltage drop for the beam, and the average energy  $\langle U^+ \rangle$  deposited into the electron gas (defined originally in Eq. (69)) is given by the weighted average,

$$\langle U^+ \rangle \sum_i \sigma_i^+[X_i] = \sum_i [X_i] \int_0^\infty du u \sigma_i^+(u). \quad (105)$$

Cross section data for high-energy electron beam excitation has been given by Berger and Seltzer<sup>23</sup>. If multiple scattering effects are important for the physical problem to be analyzed, the Berger-Seltzer

cross sections can be appropriately adjusted by multiplying by some scale factor to produce an effectively larger deposition. The present analysis requires, as input rate constants, the total scattering cross sections  $\sigma_i^*$  and  $\sigma_i^+$  for the  $e^-$ -beam collision processes. In the case of excited state production, the information provided by  $\sigma_i^*$  is sufficient. However,  $e^-$ -beam ionization processes must be included in the source term (70) to the Boltzmann equation, and therefore, the detailed energy dependence of the cross section  $\sigma_i^+(u)$  is required. For simplicity, it shall be assumed that the shape of the energy dependence is the same for all processes, so that the source term given by Eq. (70) can be written

$$S(u) = (J_b/e) \sum_i \sigma_i^+ N_i s(u), \quad (106)$$

where  $s(u)$  is a normalized shape function satisfying

$$\int_0^\infty du s(u) = 1. \quad (107)$$

Thus, the average energy  $\langle U^+ \rangle$  deposited as electron kinetic energy is

$$\begin{aligned} \langle U^+ \rangle &= \frac{\int_0^\infty du u s(u)}{\int_0^\infty du s(u)} \\ &= \int_0^\infty du u s(u). \end{aligned} \quad (108)$$

The total rate of creation of secondary electrons by  $e^-$ -beam ionization ( $\text{cm}^{-3}/\text{s}$ ) is thus



$$S_b = \int_0^{\infty} du S(u) = (J_b/e) \sum_i \sigma_i^+ N_i \int_0^{\infty} du s(u) = (J_b/e) \sum_i \sigma_i^+ N_i, \quad (109)$$

as given by Eq. (68), and the energy deposition rate (i. e., power density,  $W/cm^3$ ) is

$$\int_0^{\infty} du (eu) S(u) = e S_0 \int_0^{\infty} du u s(u) = e \langle U^+ \rangle S_b, \quad (110)$$

where  $e = 1.602 \times 10^{-19}$  J/eV. For convenience, the normalized shape function  $s(u)$  is defined (by input) to be a square wave,

$$s(u) = \begin{cases} 0, & u < u_a, \\ 1/(u_b - u_a), & u_a \leq u \leq u_b, \\ 0, & u > u_b, \end{cases} \quad (111)$$

and thus,

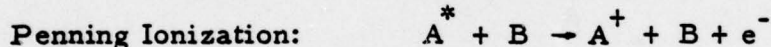
$$\langle U^+ \rangle = (u_a + u_b)/2. \quad (112)$$

Because the present approach to  $e^-$ -beam deposition is phenomenological with no a priori knowledge of energy dependence, the simplified assumptions for  $s(u)$  must suffice. Furthermore, it should also be noted that the present formulation of  $e^-$ -beam excitation and ionization collisions does not provide an explicit mechanism for heating the gas by direct deposition into molecular kinetic energy. The phenomenological description of  $e^-$ -beam deposition should be sufficiently flexible to be applicable to typical situations of interest. Where the approximations are inadequate, the analysis must necessarily be extended as required.

## Secondary Electron Creation

In addition to  $e^-$ -beam ionization, there are a variety of kinetic mechanisms which involve the creation of secondary electrons. It is appropriate to make some comments here with regard to the manner in which such processes are to be included in the Boltzmann analysis, and to discuss the resulting consequences for the power balance equation.

In general, any kinetic reaction which involves the creation of secondary electrons must be accounted for in the source term  $S_{\text{ext}}(u)$  for the Boltzmann equation. The contribution of  $e^-$ -beam ionization to  $S(u)$  is given by Eq. (106). Other electron creation processes could include, for example,



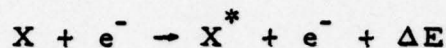
Since there is no a priori knowledge of the kinetic energy distribution of the created secondary electrons, it is convenient to assume that they are all created at zero energy and that the remaining energy  $\Delta E$  is converted to molecular kinetic energy. (This is analogous to the treatment of electrons created by secondary ionization.) The contribution from such processes to the source term is proportional to a  $\delta$ -function:

$$S_{\text{ext}}(u) = (J_b/e) \sum_i \sigma_i^+ N_i s(u) + \delta(u) \left[ I \sigma_{\text{ph}}[A]/h\nu + \right. \\ \left. + I \sigma_{\text{pd}}[A^-]/h\nu + k_{\text{PI}}[A^*][B] + \dots \right] \quad (113)$$

The  $\delta$ -function term makes no contribution to electrical power balance.

## Secondary Electron Collisions

For a binary electron-molecule collision,



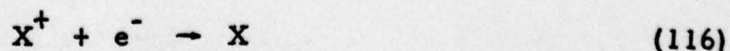
the energy  $\Delta E$  is given by  $\Delta E = -eu^*$ , where  $u^*$  is the inelastic energy loss (eV) for the process. Thus, the contribution of secondary electron collisions to the right hand side of the molecular power balance Eq. (5) is

$$-\sum_{\alpha} R(\alpha) \Delta E(\alpha) = n_e \sum_{\alpha} (eu_{\alpha}) \left[ N_{\alpha} \langle v Q_{\alpha} \rangle - N_{\alpha}^* \langle v Q_{-\alpha} \rangle \right] \quad (114)$$

Note that the sum on the right hand side of Eq. (114) is not restricted to exclude attachment (or recombination) processes, as was the case in Eq. (67) for electrical power balance. For attachment and recombination, denoted by "a", the difference

$$\begin{aligned} n_e N_a e(2e/m)^{1/2} \int_0^{\infty} du u^2 f_0(u) Q_a(u) - n_e N_a (eu_a) \langle v Q_a \rangle \\ = n_e N_a e(2e/m)^{1/2} \int_0^{\infty} du u(u - u_a) f_0(u) Q_a(u) \end{aligned} \quad (115)$$

can be interpreted as (a contribution to) the kinetic heating of the molecular gas mixture. For example, in a "two-body" recombination process such as





the ionization energy  $u^+$  and the electron kinetic energy are converted to kinetic energy of X and to recombination radiation energy  $u_r = h\nu_r$  of a photon (which has been tacitly suppressed in (116)). Since  $u_a (= -\Delta E) = -u^+$  for reaction (116), the resulting power density is

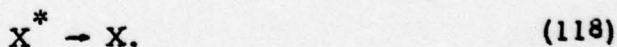
$$P = en_e[X^+](2e/m)^{1/2} \int_0^\infty du u \left[ (u + u^+ - u_r) + u_r \right] f_0(u) Q_r(u), \quad (117)$$

where  $Q_r(u)$  is the recombination cross section. The first term represents conversion of energy to molecular kinetic energy, and the second to radiation. In the subsequent discussion, we shall neglect the distinction, and simply interpret Eq. (117) as molecular kinetic heating.

### Radiative Processes

Both spontaneous as well as stimulated emission and absorption processes can be included in the present analysis. In addition to stimulated processes involving the laser transition, absorption of laser radiation by other species may also occur. There are certain distinctions and conventions that must be observed in the present analysis, and the corresponding interpretations for the power balance equation will be discussed.

First of all, spontaneous emission photons (except for those which build up the laser field) are neglected as independent species in the reaction syntax, specified by



The contribution of this reaction to the right hand side of Eq. (5) is just

$$- R\Delta E = - eu^*[X^*] / \tau_{sp} \quad (119)$$

where  $\Delta E = e u^*$  is the energy defined by Eq. (6), and  $\tau_{sp}$  is the spontaneous radiative lifetime. For all of the spontaneous emission processes from excited states, the terms of the form (119) can be interpreted as fluorescence loss. The syntax of Eq. (118), which explicitly omits reference to the radiated photon, is recognized by the computer analysis to represent spontaneous emission.

For the photon field of the laser, however, the syntax for defining spontaneous radiation is



where the emitted photon must be explicitly indicated. The reason for this is that the laser field is defined in terms of the intracavity photon number density, and laser photons are treated as species on an equal basis with electrons, ions, molecules, and all of the other "particle" species which occur in the kinetic reaction scheme. To insure a parallel treatment, some further observations and definitions must be made.

First of all, since the volume of the active gain medium is less than the cavity volume by a factor  $(L_g/L_c)$ , it is appropriate to define

$$N_{ph} = (L_c/L_g) n_{ph} \quad (121)$$

as an effective photon number density in the gain medium (as if the radiation were considered to be confined to the gain volume). This is logical, since the power balance Eq. (5) is formulated in terms of the power density in the gain medium, and all of the other species are described by their population densities in the gain medium. In terms of the photon

density  $N_{ph}$ , the intracavity intensity is

$$I = (L_g/L_c) c h \nu N_{ph}, \quad (122)$$

and the radiation Eq. (13) becomes

$$dN_{ph}/dt = (\Omega/4\pi) N^*/\tau + (L_g/L_c) c [\alpha(t) - \alpha_{th}] N_{ph}. \quad (123)$$

$\alpha(t)$ , the instantaneous net gain coefficient, was defined in Eq. (10), and  $\alpha_{th}$  is the threshold loss coefficient, given by

$$\alpha_{th} = [\gamma + (1/2) \ln(1/R)] / L_g, \quad (124)$$

where  $\gamma$  is the intracavity loss per pass (i.e. from optical elements), and  $R$  is the output coupling reflectivity. The total contribution from output coupling and the radiative processes of Eq. (7), (8), and (120) to the power balance equation (5) is

$$\begin{aligned} & \sum_A E_A d[A]/dt + \sum_{A^*} E_{A^*} d[A^*]/dt + h\nu dN_{ph}/dt \\ & + E_{X^*} d[X^*]/dt + E_X d[X]/dt = - [1 - (\Omega/4\pi)] [X^*] h\nu/\tau \\ & - (I/h\nu) \sum_A \sigma_A [A] (E_A - E_{A^*} + h\nu) - I \alpha_{th} \end{aligned} \quad (125)$$



The interpretation of the terms of Eq. (125) is straightforward. On the left hand side, there is the rate of change of stored energy density. The first term on the right hand side represents the net fluorescence power loss from reaction (120), and is consistent with the assumption that a fractional part ( $\Omega/4\pi$ ) of the spontaneous emission photons are not lost, but remain in the cavity to build up the optical field. Reference to Eq. (8) shows that the energy difference ( $E_A + h\nu - E_{A^*}$ ) corresponds to the net energy converted to kinetic energy of the species  $A^*$ . Thus, the second term on the right hand side of Eq. (125) can be interpreted as a kinetic heating power density. The third term corresponds to optical loss, due to absorption by intracavity optical elements ( $\gamma$ ), and output coupling ( $R$ ).

#### Kinetic Heating

With the exceptions noted above, the energy change  $\Delta E$  defined by Eq. (6) for the reaction (1) is the net energy converted to molecular kinetic energy, and thus, the physical significance of the term

$$\sum_{\beta} R(\beta) \Delta E(\beta)$$

on the right hand side of Eq. (5) is that it represents power density into kinetic heating of the molecular gas. The exceptions which occurred were the result of the tacit suppression of some species involved (e.g., the emitted photon in spontaneous radiation) or of the kinetic energy dependence of some of the interacting species (e.g., secondary and high-energy  $e^-$ -beam electrons). In the case of secondary electrons, for which an integration over a continuum of energies is required, the contribution to the power balance must be derived from the Boltzmann equation.

### Total Power Balance for the Coupled System

As a result of the foregoing discussion, which should clarify the physical significance of the terms of Eq. (5), it is now possible to construct the equation for conservation of power density for the coupled system of electrons, molecules, radiation, and external driving circuit. If Eq. (5) is added to the expression given by Eq. (67) for  $e\bar{u}dn_e/dt$ , and the terms are rearranged, the following result is obtained:

$$\begin{aligned}
 & \sum_i E_i d[X_i]/dt + h\nu dN_{ph}/dt + e\bar{u}dn_e/dt + \sum_A h\nu_A [A^*]/\tau_A \\
 & + \left[1 - (\Omega/4\pi)\right] h\nu [X^*]/\tau + I\alpha_{th} + \sum_{\beta}' R(\beta)\Delta E(\beta) \\
 & + en_e \sum_{a,r} N_a \left[ (2e/m)^{1/2} \int_0^{\infty} du u^2 f_o(u) Q_a(u) - u_a \langle v Q_a(u) \rangle \right] \\
 & + en_e (2e/m)^{1/2} \int_0^{\infty} du u^2 \langle (2m/M) N Q_m \rangle \left[ f_o + (kT/e) df_o/du \right] \\
 & = \sigma E^2 + J_b \sum_k \left[ u_k^* \sigma_k^* + [u_k^+ + \langle U^+ \rangle] \sigma_k^+ \right] [X_k] \\
 & = \sigma E^2 + J_b dV/dx. \tag{126}
 \end{aligned}$$

The first three terms on the left correspond to the rate of change of the energy density stored in the molecules, radiation field, and electrons. The sum over  $i$  excludes electrons, but photons (which have been shown explicitly in the second term) could be included in that sum by defining

$E_i = h\nu$  for that "species". The fourth and fifth terms represent spontaneous fluorescence loss, while the sixth is the optical power loss by intracavity absorption and output coupling. The remaining terms on the left hand side have the significance of kinetic heating of the molecular gas. The sum over  $\beta$  in the seventh term includes all processes except spontaneous emission, secondary electron collisions, and high-energy  $e^-$ -beam collisions. All resonant energy transfer processes (i. e. for which  $\Delta E = 0$ ) contribute nothing to the sum over  $\beta$ , nor does the stimulated emission reaction, since  $\Delta E = E_{X^*} - E_X - h\nu = 0$ . The eighth term consists of the net contribution to molecular heating from recombination and attachment processes, assuming that recombination radiation is neglected. The last term on the left hand side is the power density into elastic heating from electron-molecule momentum transfer collisions.

On the right hand side, there is the input electric discharge power density  $\sigma E^2$  and the beam deposition  $J_b dV/dx$ , where the effective  $e^-$ -beam voltage drop  $dV/dx$  was defined in Eq. (104). The discharge power density  $\sigma E^2$  can be expressed in terms of the parameters of the external driving circuit by Eq. (99).

In its present formulation, the coupled analysis assumes that the molecular temperature of the gas remains constant. This restriction could easily be removed, if necessary, by an additional equation

$$C_v dT_{\text{mol}}/dt = \sum_{\beta} R(\beta) \Delta E(\beta) + \text{misc. heating terms} \quad (127)$$

where  $C_v$  is the specific heat of the gas at constant volume ( $J/cm^3 K$ ), and the right hand side is the total power density into kinetic heating.



The numerical solution of the coupled system of molecular and electron kinetic equations proceeds as follows. The total pulse duration is divided into a specified number (e.g., 200) of (equal) subintervals defined by a time grid  $[0, t_1, t_2, \dots, t_k, \dots]$ . At each of the discrete points  $t_k$  in time, the Boltzmann equation is solved (as a function of the instantaneous values  $E(t_k)/N$  and the excited state population densities  $N_\alpha(t_k)$ ) to update the electron excitation rates  $\langle vQ_\alpha \rangle$  and plasma parameters, which are then assumed to remain constant over the following subinterval  $[t_k, t_{k+1}]$  of time. The molecular kinetic (and circuit) equations are integrated over this subinterval, and in practice, the integration step size will usually be much smaller than the coarse time intervals  $[t_k, t_{k+1}]$  over which the electron kinetics calculations are performed. The Gear<sup>6</sup> technique automatically adjusts the step size to maintain accuracy and stability.

The assumption that the electron energy distribution function  $f_0(u)$  is constant over these discrete subintervals will result in a power balance discrepancy in the calculations. Assume that  $f_0^k(u)$ ,  $\langle vQ_\alpha \rangle_k$ ,  $\mu_k$ ,  $\bar{u}_k$ , ... represent the electron distribution, excitation rates, mobility, average energy, etc. obtained from solution of the Boltzmann equation at some discrete point  $t = t_k$ . If Eq. (67) were to be numerically evaluated at a later time  $t$  by the approximations that  $f_0(u) = f_0^k(u)$ ,  $\langle vQ_\alpha \rangle = \langle vQ_\alpha \rangle_k$ ,  $\bar{u} = \bar{u}_k$ ,  $\mu = \mu_k$ , ... the right hand side would contain an additional term  $\delta P$  representing a power discrepancy:

$$\begin{aligned} \delta P(t_k, t) = & e n_e(t) \mu_k E(t)^2 + e \langle U^+ \rangle S_b(t) - e \bar{u}_k dn_e(t)/dt \\ & - n_e(t) e (2e/m)^{1/2} \int_0^\infty du u^2 \langle (2m/M) N Q_m \rangle \left[ f_0^k(u) + (kT/e) df_0^k(u)/du \right] \end{aligned}$$

(continued)

$$\begin{aligned}
& - n_e(t) \sum_{\alpha} (eu_{\alpha}) \left[ N_{\alpha}(t) \langle v Q_{\alpha} \rangle_k - N_{\alpha}^*(t) \langle v Q_{-\alpha} \rangle_k \right] \\
& - n_e(t) e(2e/m)^{1/2} \sum_a N_a(t) \int_0^{\infty} du u^2 f_0^k(u) Q_a(u). \quad (128)
\end{aligned}$$

Since  $f_0^k(u)$  and the corresponding plasma parameters and excitation rates are recalculated at the point  $t_{k+1}$ , the longest period of time over which the approximation  $f_0(u) = f_0^k(u)$  is sustained is the length of the discrete interval,  $\Delta t = t_{k+1} - t_k$ . Therefore, a useful measure of the accuracy of the calculation (at least insofar as it is affected by errors resulting from the discrete time partition) should be

$$\xi(t_k, t) = P(t_k, t) / P_{\text{tot}}(t), \quad (129)$$

where

$$P_{\text{tot}}(t) = en_e(t) \mu(t) E(t)^2 + J_b(t) dV/dx \quad (130)$$

is the total electrical input power density. If Eq. (128) is evaluated at the time  $t = t_k$ , a measure of power balance inaccuracy resulting from the numerical solution of the Boltzmann equation is obtained. (Since it is only the contribution  $e \langle U^+ \rangle S_b$  to  $J_b dV/dx$  that occurs in the electron kinetics analysis, the fractional power discrepancy reported from the Boltzmann calculations is normally defined in terms of total electrical excitation power density,

$$P_e = en_e \mu E^2 + e \langle U^+ \rangle S_b. \quad (131)$$

The present formulation of the coupled system of equations makes the

tacit assumption that the charge  $q(t)$ , current  $i(t)$ , and all of the population densities  $N_\alpha(t)$  are continuous from  $t_k^- = t_k - 0$  to  $t_k^+ = t_k + 0$ :

$$\begin{aligned} i(t_k^-) &= i(t_k^+), \\ q(t_k^-) &= q(t_k^+), \\ N_\alpha(t_k^-) &= N_\alpha(t_k^+), \end{aligned} \tag{133}$$

and thus, these quantities can always be defined unambiguously as functions of the time  $t_k$ . However, all of the electron parameters and excitation rates are discontinuous from  $t_k^-$  to  $t_k^+$ , since they are updated at  $t = t_k$  by a new solution of the Boltzmann equation. Furthermore, the derivatives  $di(t)/dt$ ,  $dn_e(t)/dt$ , and  $dN_\alpha(t)/dt$  for all species  $\alpha$  which are involved in secondary electron collision processes will also be discontinuous. At  $t = t_k^-$ , just prior to the Boltzmann update, the electric field is obtained from

$$E_k = E(t_k^-) = i(t_k^-)R_d(t_k^-)/d = i(t_k^-)/[Aen_e(t_k^-)\mu(t_k^-)], \tag{134}$$

and the fractional power discrepancy  $\xi(t_k, t_k)$  defined by Eq. (128) and (131) is based upon the assumption that  $E_k$  is the electric field. However, the plasma conductivity  $\sigma = en_e\mu$  (and thus, the discharge impedance  $R_d = d/A\sigma$ ) are discontinuous from  $t_k^-$  to  $t_k^+$ , and therefore, the electric field at  $t = t_k^+$  is

$$E_k^+ = E(t_k^+) = i(t_k)/[Aen_e(t_k)\mu(t_k^+)] = (\mu_k^-/\mu_k^+)E_k. \tag{135}$$

Thus, in addition to the power discrepancy  $\delta P(t_k, t_k)$  inherent in the numerical solution of the Boltzmann equation, there will also be an imme-



diate discrepancy associated with the discontinuity in the electric field:

$$\begin{aligned}\delta P(t_k, t_k^+) &= \delta P(t_k, t_k) + en_e(t_k) \mu(t_k^+) [(E_k^+)^2 - E_k^2] \\ &= \delta P(t_k, t_k) + en_e(t_k) \mu_k^+ E_k^2 [(\mu_k^-/\mu_k^+)^2 - 1],\end{aligned}\quad (136)$$

where  $\mu_k^+ = \mu(t_k^+)$ . There are three fractional power discrepancies which are a useful measure of the accuracy of the calculations. The first is the inherent power accuracy of the numerical solution of the Boltzmann equation,

$$\xi_k^0 = \delta P(t_k, t_k)/P_e, \quad (137)$$

and it is provided as part of the output summarizing the results of the electron kinetics analysis. The second is

$$\xi_k^- = \xi(t_{k-1}, t_k^-) = \delta P(t_{k-1}, t_k^-)/P_{\text{tot}} \quad (138)$$

which represents the cumulative error which has developed over the entire preceding subinterval of time. The third is

$$\xi_k^+ = \xi(t_k, t_k^+) = \delta P(t_k, t_k^+)/P_{\text{tot}} \quad (139)$$

which represents the fractional additional error resulting from discontinuity in the electric field before and after the Boltzmann update. If  $\xi_k^+$  or  $\xi_k^-$  are too large, the length  $\Delta t = t_{k+1} - t_k$  of the subintervals should be reduced.

### 3.0 COMPUTER PROGRAM DESCRIPTION

The generalized laser kinetics code has been written in FORTRAN IV, and was developed for use with the Extended FORTRAN Compiler of the CDC 6000 and CYBER Series of computers (SCOPE 3.4). If it is necessary to execute this program on a different computer system, some modifications of nonstandard syntax or conventions may be required. In addition, extensive usage of ENCODE and DECODE statements (for output formatting) makes the explicit assumption that the basic "word" size is 60-bit, 10-BCD character display. Modification of such statements will be necessary if the program is to be adapted to a computer with a different word size.

The program structure, flow diagrams, description of subroutines, control card commands and requests, external file usage, input card format and default conditions, available output options, and illustrative input and output from a sample case will all be described. The complete FORTRAN program listing is given in Vol. II of the present report. In addition, Vol. II also contains a listing for an electron kinetics analysis program, which makes use of the same subroutines.

#### 3.1 Program Structure and Flow Diagram

The program structure has been designed with the objective of providing maximum input and output flexibility, while reducing mechanical programming tasks for the user to a minimum. A given kinetic reaction scheme is specified by input (with a completely free and flexible syntax) as a sequence of symbolic reactions containing an arbitrary number of processes and interacting species. These reactions are translated into computer-coded FORTRAN equations to generate molecular kinetics subroutines, which are then combined with the master

executive program LASER and (seventeen) other subroutines to form a completely self-contained source program for the coupled analysis based upon the specified reaction scheme (cf. Fig. 2.3).

Fig. 3.1 presents a more detailed flow diagram of the main program LASER. Initially, there may or may not be a synthesized program available, and the control cards and data input deck structure must be compatible so that LASER can execute either situation. Initially, the program makes an attempt to read "TITLE" on an attached file TAPE4, which would normally contain the "name" and miscellaneous rate constant data associated with a synthesized reaction scheme of a previous run. If an EOF is encountered on the attempt to read file TAPE4, the program assumes that user intends to generate subroutines and a data file for a new reaction scheme, to be specified by input DATA BLOCK 1. In that case, the input of DATA BLOCK 1 is processed by Subroutine SYNTH, which translates the reaction structure into three subroutines (DNDT, JACOB, and LEVELS) which consist of 80-BCD character records on file MTAPE (= 3). Furthermore, as the reaction scheme of DATA BLOCK 1 is processed, miscellaneous data is written onto file TAPE4. Diagnostics are generated for a variety of error conditions which may be encountered. Although synthesis proceeds by ignoring unacceptable syntax or other errors, protection against subsequent execution of a faulty reaction scheme can be obtained by declaring such conditions to be fatal. After files TAPE4 and TAPE3 are constructed, EXIT occurs, the synthesized subroutines are compiled and combined with the other subroutines, and LASER is again executed. This time, TAPE4 contains reaction scheme data, and the attempt to read "TITLE," the "name" of the synthesized program, is successful. Control transfers to Read DATA BLOCK 2, which contains input electron cross section data.



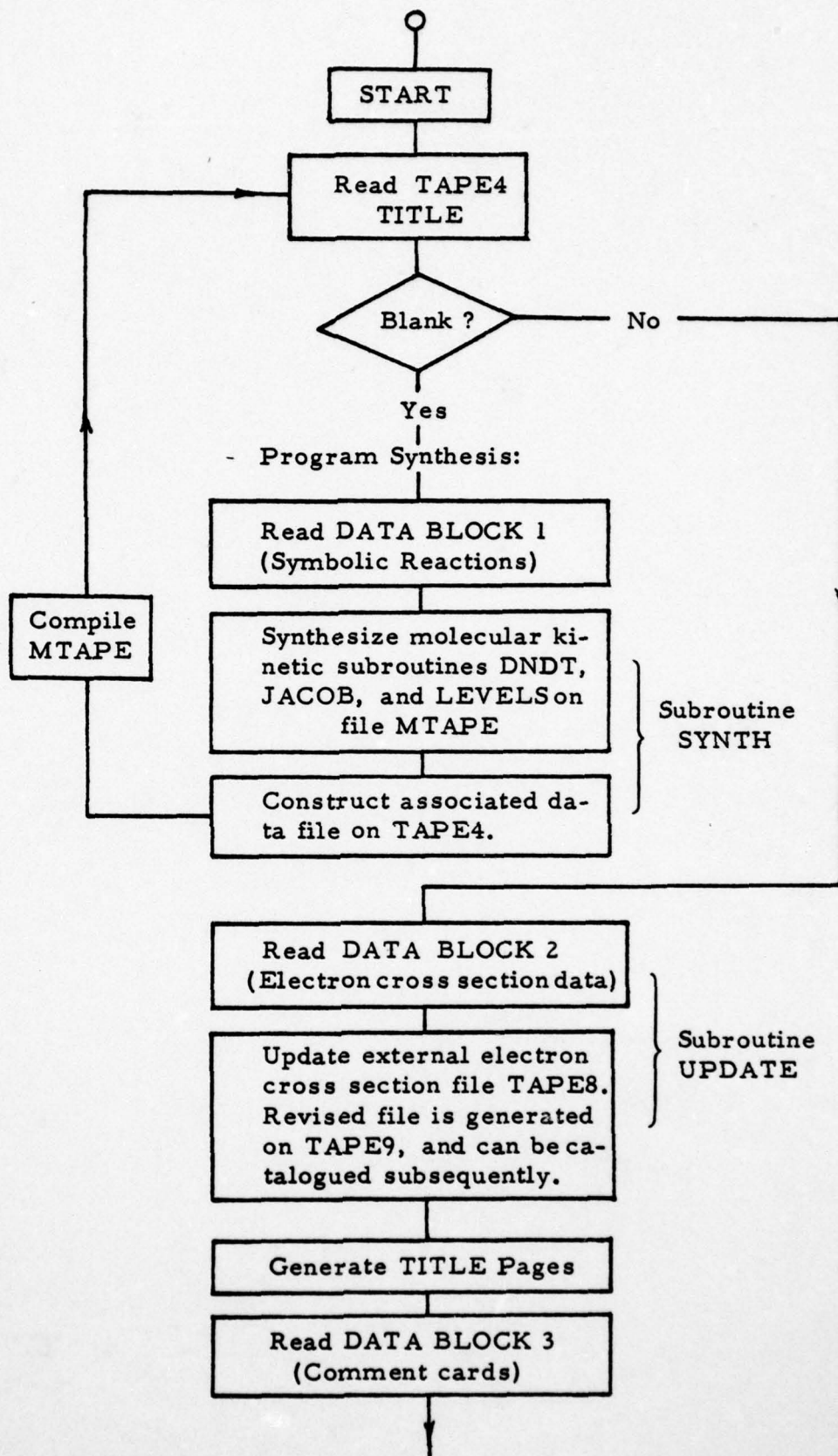


Fig. 3.1: Flow diagram of LASER Synthesis Code.

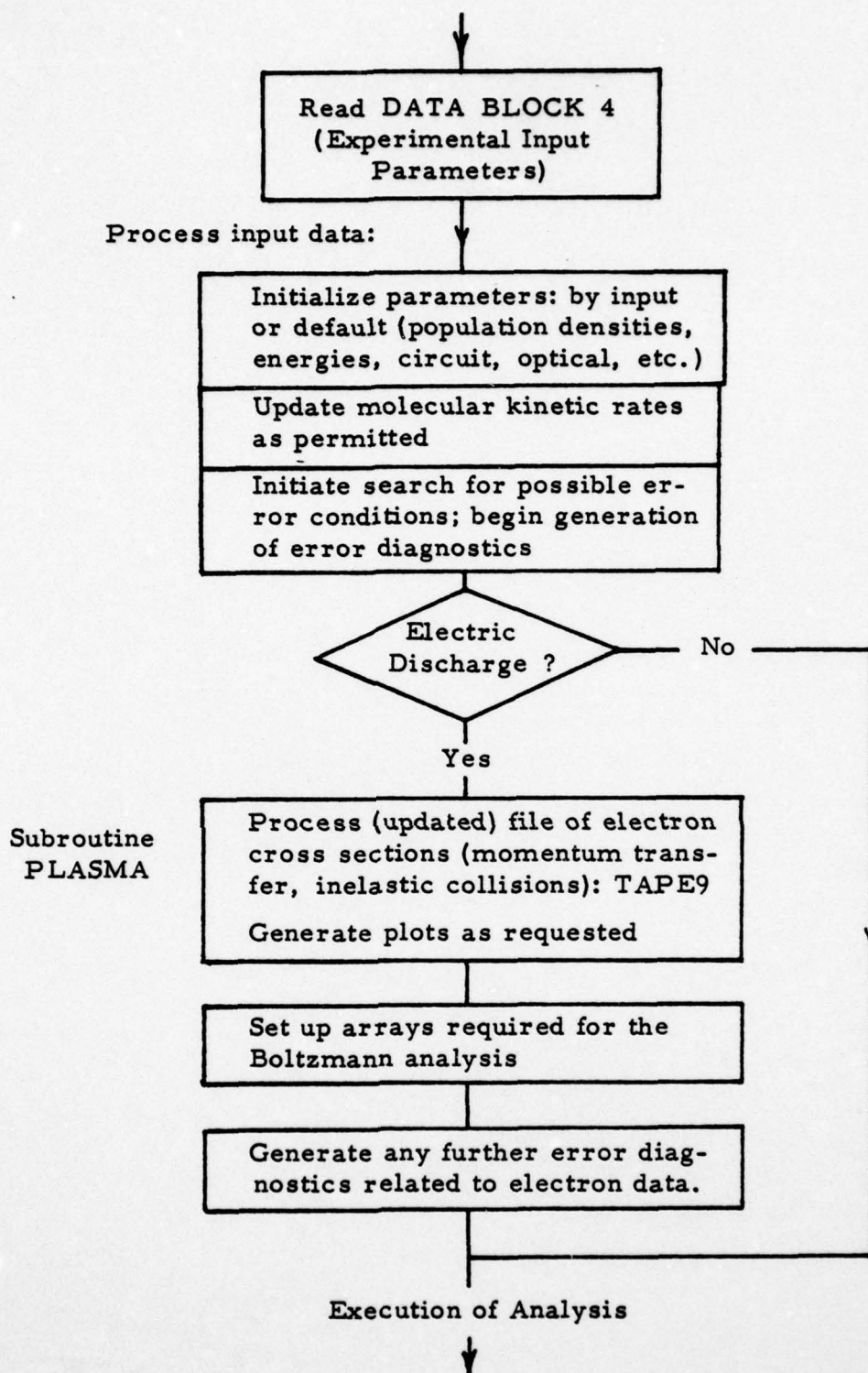


Fig. 3.1: Flow Diagram of LASER Synthesis Code (cont'd).

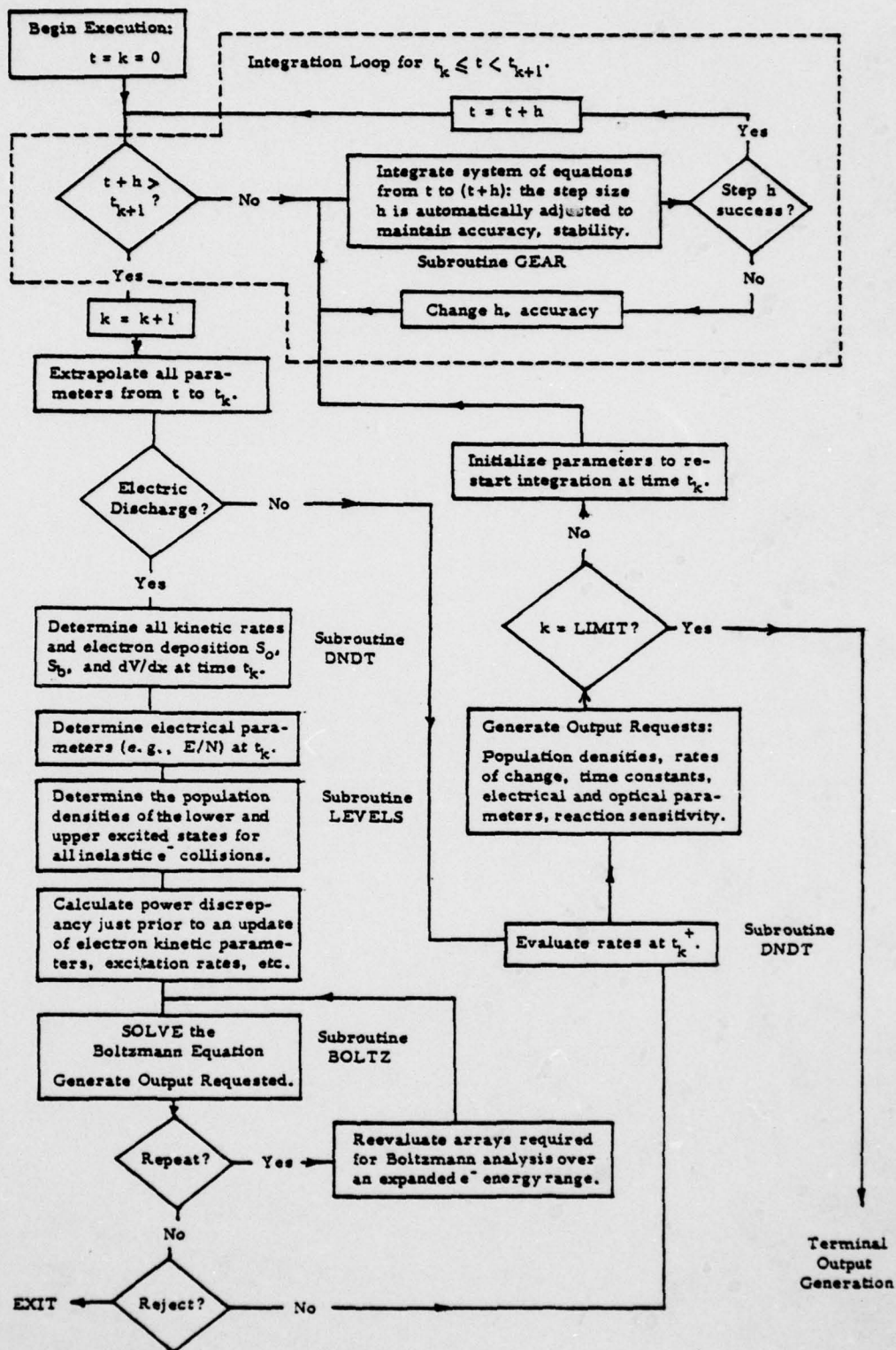


Fig. 3.1: Flow Diagram of LASER Synthesis Code (cont'd).



Electron cross section card data is entered by DATA BLOCK 2 to update a main electron cross section library, which is provided on file TAPE8. The updated library, which is generated on TAPE9, may be catalogued for future use if desired. DATA BLOCK 2 may be completely empty, or it may contain extensive data; indeed, the initial library itself can be constructed by "updating" an empty file on TAPE8 and cataloging the resulting TAPE9. During subroutine synthesis and reaction processing, a search is made (for each secondary electron collision encountered) to determine whether the appropriate cross section data is available in the external library. If it is not, a warning diagnostic is generated. The only cross section data available at the time of program synthesis is the original data on TAPE8. An omission error, which would most likely be declared fatal initially, could always be removed by an electron file update on a subsequent run.

DATA BLOCK 3 contains comment cards which are reproduced in the output. DATA BLOCK 4 contains the experimental input parameters for execution of the analysis. The input data is processed and all of the run parameters are initialized (explicitly or by default). The molecular kinetic rate constants are updated, as permitted.

At the time of subroutine synthesis, reactions are defined by their forward and reverse rate constants. If a rate constant (e.g., for the reverse reaction) was zero, no translation of that term occurs and no subsequent modification of that rate is accessible to input. For secondary electron collisions, however, the appearance of a zero rate constant automatically produces a default to the Boltzmann analysis. If a nonzero rate constant was initially provided (at the time of synthesis) for a secondary electron process, no coupling of that process to the Boltzmann analysis occurs. No subsequent modification of a rate

constant which defaults to the Boltzmann analysis is permitted. An exception occurs for the situation of no electric discharge, in which case, input modification of a secondary electron rate is accepted. A detail balance relation is enforced for binary collisions, with the reverse rate defined in terms of the product of the forward rate and an exponential factor. Therefore, reverse rate constants for such processes cannot be modified either. An illegal attempt to modify rates inaccessible to input in DATA BLOCK 4 is detected (and ignored) and an error diagnostic is generated.

The analysis is executed by subdividing the total pulse time TPULSE into NCYCLE (equal) subintervals of time  $\Delta t = \text{TPULSE}/\text{NCYCLE}$ , defining a partition of discrete times  $t_k = k\Delta t$  ( $k = 0, 1, 2, \dots, \text{LIMIT}$ ). At each of these discrete times, the Boltzmann equation is solved to update the electrical parameters and electron excitation rates, and a variety of output option requests can be specified. Normally, TPULSE is the total pulse interval, and  $\text{LIMIT} = \text{NCYCLE}$ ; however, the combination of parameters TPULSE, NCYCLE, and LIMIT provides more flexibility for the joint specification of total integration time and the frequency of electron kinetic updates and output generation. Over the subinterval  $t_k \leq t < t_{k+1}$ , the coupled molecular and circuit equations are integrated using a multistep Gear technique<sup>6</sup>, shown in the dashed box in Fig. 3.1. If the current integration step size is  $h$  and the time is  $t$ , the program tests whether an additional integration to time  $(t + h)$  would exceed the next cycle time  $t_{k+1}$ ; if so, program resets the cycle count to  $(k + 1)$  and extrapolates all parameters from time  $t$  to time  $t_{k+1}$  by the use of an array (provided by Subroutine GEAR) which contains population densities and their derivatives (to various orders). If  $(t + h)$  would not have exceeded the next discrete cycle point, the GEAR subroutine continues the integration across the



subinterval. Subroutine GEAR automatically adjusts the step size  $h$  to maintain accuracy and stability.

If the amount of time consumed by the Boltzmann updates and output generation at a cycle time  $t_k$  were negligible, the total CP time for execution of the complete analysis should be independent of NCYCLE, since the integration would only be interrupted by brief pauses at  $k = 0, 1, 2, \dots$ . In actual fact, these additional tasks performed at the cycle times  $t_k$  do consume only a small fraction of the total computation time for integration from  $t_k$  to  $t_{k+1}$ . However, it has been observed (from actual runs of the program) that the total CP execution time seems to increase proportionately with (rather than be relatively independent of) NCYCLE. At the discrete time  $t_k$ , after the electron kinetic calculations and output generation, the GEAR integration must be restarted (with JSTART = 0). For the case of an electric discharge, some of the kinetic rate constants (i. e., those for the secondary electron collisions) change from  $t = t_k^-$  to  $t = t_k^+$ , and it is possible that the restart process consumes an excessive time before the step size can be finally increased to its most economical size. So long as the integration loop in the dashed box is not disturbed, execution is efficient and an economically large step size is attained and maintained. However, an exit and subsequent return to the integration loop with a restart seems to cause the problem. (The problem does not seem to arise for calculations involving no electric discharge.) There has not been adequate opportunity to explore conclusively the origins of this difficulty, or to optimize the execution time. However, it is quite likely that significant improvement in execution efficiency should be possible with only minimal modifications in the integration technique. In any case, for the present version of the program, it is advantageous to use a relatively small (e.g., 50, 100) value of NCYCLE.



After  $k = \text{LIMIT}$  is attained, execution terminates and control is transferred to final output generation. This includes miscellaneous tables and plots of electrical and optical quantities, molecular population densities, etc. as a function of time.

The listing of the program, which appears in Vol. II, contains extensive COMMENT card documentation of additional information which is too detailed to be described here. As most of the FORTRAN variable names have been chosen to be reasonably descriptive of the physical quantities they represent, it is believed that the logical and computational structure of the program should be relatively straightforward when supplemented with Fig. 3.1 and the present discussion.

The program has been written in such a way that dimension storage can be changed relatively easily. Arrays are communicated to subroutines by variable dimension calls and thus, it is sufficient to define a set of DIMENSION declarators which can be easily modified. The DIMENSION statement changes required are described by COMMENT cards in the listing. The only other precaution that must be observed is that labelled COMMON blocks shared with subroutines synthesized in previous runs must be consistent.

External file usage (TAPE2, TAPE3, ..., TAPE10) is as follows: TAPE2 is a scratch file used in subroutine synthesis and analysis of reaction sensitivity. TAPE3 and TAPE7 are used for writing the FORTRAN translation of the symbolic reaction scheme; they are subsequently combined on TAPE3, which provides a source file of 80-BCD character records of the statements of the synthesized subroutines JACOB, DNDDT, and LEVELS which can be compiled. TAPE4 is a file provided for writing miscellaneous reaction data associated

with a specified kinetic scheme. TAPE4 contains data which is an essential supplement to the synthetically generated program, and it must be catalogued and saved if future execution is intended. TAPE3 (which consists of 80-BCD character records which are the FORTRAN statements of the synthesized subroutines) can be used as the input source for creation of an UPDATE program library, which can be catalogued and saved if any future specialized modifications (beyond the scope of the synthesis capability of LASER) are anticipated. Normally, it would be sufficient to catalog and save the binary compilation of subroutines DNDT, JACOB, and LEVELS for future execution. Thus, even for specialized situations for which LASER may not be totally adequate for synthesizing the exact structure desired for the rate subroutines, it is always possible to revise the source program generated by means of subsequent update procedures.

TAPE8 is used for an attached file of electron cross section data. The electron cross section library can be updated by DATA BLOCK 2 card input to form a revised file on TAPE9, which can be catalogued and saved for future use as desired. TAPE10 is the card input file; a processing subroutine EDITOR reads card input data to an EOF on unit 10 and generates an output playback of the card images. It also copies the card images onto TAPE5, creating an effective card input file on unit 5. Each time a new data block (terminated by an EOF card) is encountered, playback of card images and creation of an effective input file TAPE5 occurs. TAPE6 is used for OUTPUT.

In the following sections, some of the important subroutines will be discussed in more detail. The card format for the input data decks will be described, and the instructions for usage illustrated with sample control cards.



### 3.2 Input Data Description

Input to the code consists of card and/or tape (disc) data files. As the flow diagram of Fig. 3.1 indicates, there are four main blocks (DATA BLOCK 1, 2, 3, and 4) of card input; in addition, an external file (TAPE8) containing an electron cross section library may also be attached. In this section, a description of the card input sequences, with format specifications and physical units assumed, will be given. The external cross section file (attached on TAPE8) is originally created with card input from DATA BLOCK 2.

In order to provide maximum flexibility for data input with a minimum number of format restrictions, NAMELIST entry is frequently used. Various constants or experimental input parameters are initially assigned default values (or subsequently induce the program to take a suitable default action) that would be most appropriate for the user in typical problems of interest, were he to fail to define certain parameters explicitly by input. This allows for considerable abbreviation of input, since only essential variables need to be entered to specify execution conditions. At the same time, however, a wide range of variables remain accessible to input specification in case their default values are not acceptable. Input format for NAMELIST entry is very free, and eliminates the possibility of entering numerical data in an incorrect field of columns. Each of the NAMELIST sequences have been given physically descriptive names, and contain variables that specify related parameters for a particular aspect of the analysis.

In order to read data using NAMELIST, input data must be provided in a special form. The first character (column 1) on each card to be



read must be a blank. The second character on the first card (of a group of data cards) must be \$ (dollar sign) immediately followed by the NAMELIST name, which must not contain any embedded blanks. The name must be followed by at least one blank, which is followed by a string of data items separated by commas, and the end of a data sequence occurs when another \$ is encountered. Any (or all) of the variables included in the NAMELIST group can be entered (without regard to order) as specified input. The form of the data items on an input card is "A = const", where A is the FORTRAN name of a variable or subscripted array, and "const" is an integer, real, complex, or logical constant (or string of constants separated by commas if A is the name of an array). Numerous examples will occur in the sample output to be presented later.

Card input consists of four basic blocks of data to define the molecular kinetic reaction scheme and its rate constants, modifications (if any) for updating an external electron cross section file, comment cards to describe miscellaneous information for reproduction in the output, and experimental input parameters for execution of the analysis.

#### DATA BLOCK 1

DATA BLOCK 1, whose structure is shown in Table 3.1, occurs only for the initial synthesis of subroutines and generation of data file (on TAPE4) for a new molecular kinetic reaction scheme. The first card is a "header" containing three (10-BCD character) computer words which "name" the new program. They are used as a three-line title on a cover page preceding the output whenever the code is subsequently executed. Following the header card, there is an arbitrarily long se-

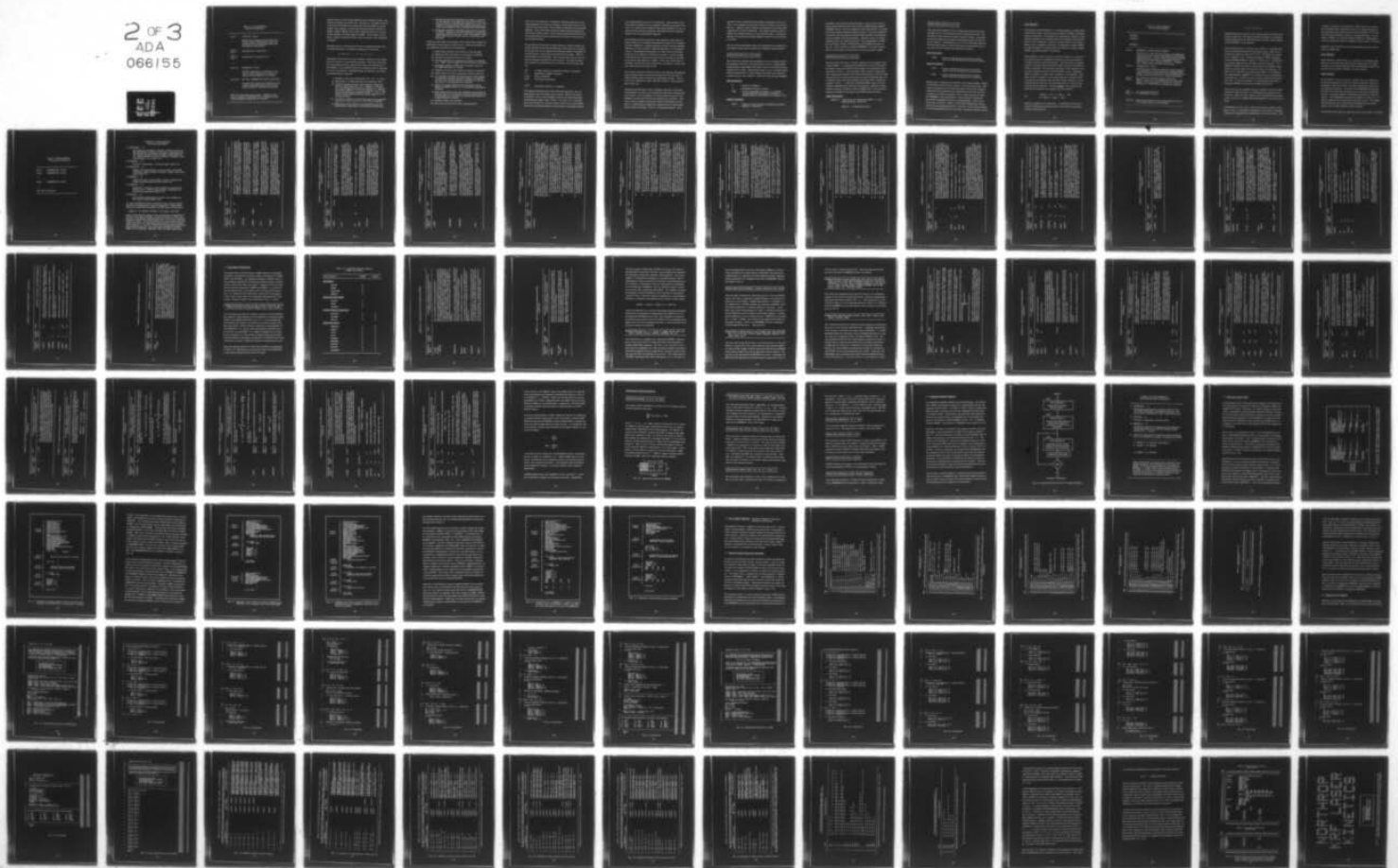
AD-A066 155

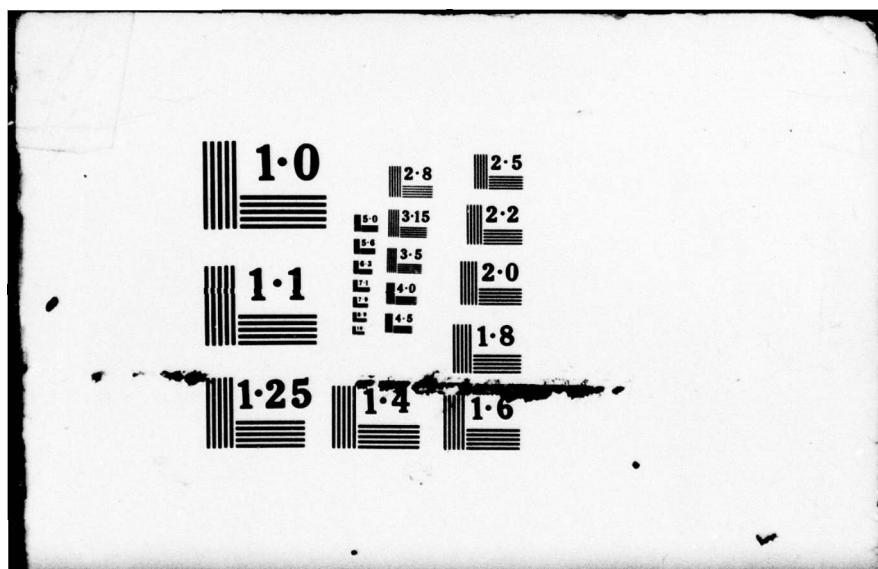
NORTHROP RESEARCH AND TECHNOLOGY CENTER PALOS VERDES --ETC F/G 20/5  
THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSES--ETC(U)  
JAN 79 W B LACINA  
N00014-78-C-0499  
NL

UNCLASSIFIED

2 OF 3  
ADA  
066155

SEE  
PAGE 1







Card 1      TITLE(3)   (3A10)

Card 2                  Specification of reaction No. 1.  
Card 3

Card 4      Specification of reaction No. 2.  
Card 5

• • • • •

Card 2n KINETIC(6) (6A10)

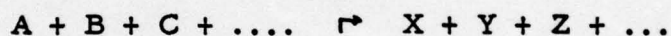
Card 2n+1    KF, KR, COMMENT(5) (2E10.3, 5X, 5A10)

- 
- 
- 
- 

91

quence of pairs of cards which define the input reaction scheme, ultimately terminated by an EOF card. (In practice, the length of the reaction queue is limited by the dimension declarator KMAX, and the number of new species encountered during processing is limited to NMAX. KMAX, NMAX, and all other dimension declarators can be easily changed in the main program LASER. If the number of reactions or species exceed the limits, they are ignored, and a diagnostic is issued.)

The first card of a reaction pair consists of a Hollerith string of up to 60 BCD characters, containing an expression of the form



The syntax for the reaction is quite flexible, allowing it to be written just as it would be in usual technical notation. Each side of the reaction may contain up to five species whose names are defined by the first NSIZE (= 10) nonblank characters recognized before a delimiter (+ or  $\rightarrow$ ) is encountered. Embedded blanks are ignored, and certain conventions must be observed:

- i) Secondary electrons are denoted by "E", "E-", or "E(-)".
- ii) High energy ( $e^-$ -beam) electrons are denoted by "HE-".
- iii) All other charged particles must explicitly exhibit their charge in their name (e.g., "F-", "KR2(+)", "AR(++)", etc.) and multiple charge must be explicit (i.e., "AR(++)" rather than "AR(2+)" ). If an ion is positive, the "+" sign must be immediately followed by another "+" or by ")" in order to avoid confusion with the normal usage of "+" in writing reactions.
- iv) Numerical coefficient in front of the species not permitted (e.g.  $A + B \rightarrow C + C$ , but not  $A + B \rightarrow 2C$ , is allowed).
- v) Buffer gases (whose identity is not important) can be denoted by "M" (resulting in a total pressure dependence).



- v) Spontaneous emission processes do not have to explicitly include a photon on the right hand side of the reaction unless the process is considered to contribute "noise" to the buildup of an optical field by stimulated amplification, in which case the photon must be included and denoted "HNU".
- vi) Stimulated emission or absorption processes are denoted by "RAD". Except for the laser transition involving stimulated emission (in which case "RAD" must appear on both sides of the reaction), "RAD" can occur only on the left hand side.

As they are processed, the reactions of the input kinetic scheme are subjected to several tests to detect errors. Among the possible error conditions encountered are the following:

- i) High energy electrons must balance on left and right.
- ii) Buffer gas "M" must balance on both sides of equation.
- iii) Charge conservation must not be violated.
- iv) Reverse processes for spontaneous emission not allowed (i.e., "HNU" must not appear on the left side of a reaction)
- v) Stimulated radiation "RAD" must not appear (alone) on the right hand side of a reaction.
- vi) Duplicate reactions (even written backward) are ignored.
- vii) Detail balance for binary molecular collisions enforced.
- viii) For secondary electron collision processes which default to Boltzmann calculation for rate constant, the attached electron cross section data file is searched to verify that appropriate cross section data is available.
- ix) Dimension storage (defined by the declarators KMAX, NMAX, and NKMAX) must not be exceeded during program synthesis.
- x) Both forward and reverse rate constants zero; reaction is ignored unless it is a secondary electron collision process, in which case rate constants are automatically linked to a coupled Boltzmann analysis.
- xi) Reaction syntax unrecognizable.
- xii) More than five species on left or right hand side.



If an error is encountered, a diagnostic warning is generated in the edited summary of reaction processing, and the faulty reaction is ignored for the construction of the synthetic subroutines and associated data file. Thus, processing continues uninterrupted throughout the entire input reaction queue, and the final program generated can even be executed unless the user declares the occurrence of such errors to be treated as fatal.

The second card in the pair of cards defining a reaction contains (an initial estimate of) the forward (KF) and reverse (KR) rate constants for the process, and an (optional) 50-character field for comments or a data reference, which will be reproduced in the output. With certain exceptions to be described, both a forward and reverse rate constant are typically provided for each reaction. The units for these rate constants are determined by the structure of the reaction, and are:

$\text{cm}^2$	$e^-$ -beam collisions; stimulated emission, absorption
$\text{s}^{-1}$	Spontaneous radiative emission
$\text{cm}^3/\text{s}$	Binary collisions
$\text{cm}^6/\text{s}$	Three-body interactions
$\vdots$	
$\text{cm}^{3n}/\text{s}$	Interaction between (n - 1) species.

The program determines the form of the rate expression, Eq. (2), automatically from the syntax of the reaction, subject to the above conventions, and it is the obligation of the user to insure that input values have the proper units. If  $KF = 0$  (or  $KR = 0$ ), no translation of the forward (or reverse) reaction term occurs in the synthesized rate subroutines and thus, null operations (containing unneces-

sary multiplications by zero) are eliminated. Rate constants used at the time of synthesis can be changed in subsequent execution, however, so a nonzero value should be used during synthesis for any reaction process (with the exception of secondary electron collisions) which is not to be permanently neglected.

For secondary electron processes, the omission of input rate constants at the time of synthesis automatically results in the linkage of the rate constants to a coupled Boltzmann electron kinetics analysis. Likewise, if a rate constant is explicitly specified, no such linkage occurs. During program generation, for those electron collisions which are to be coupled to a Boltzmann analysis, a search is made to determine if the required electron cross section data is available on the library file attached to TAPE8. If the cross section data is available, 50-character input comment is overridden by a data reference extracted from the library file.

For a binary molecular collision process, the program automatically enforces detail balance between the forward and reverse rate constants (although with no provision for degeneracy factors). The reverse rate is defined to be  $KR = KF \exp(-\Delta E/kT)$ , where  $\Delta E$  was given by Eq. (6).

Subsequent modifications of rate constants at the time of execution are permitted, but some rate constants are necessarily inaccessible to such input. If no translation of a reverse process occurred, for example, no future input of that rate constant can contribute. Likewise, if rate constants automatically default to Boltzmann calculations or a detail balance expression, opportunities for input modification cannot be provided. There is one logical exception: if the



analysis has been synthesized with default to Boltzmann electron kinetics, rate constants for secondary electron collisions can be modified (i.e., defined by input) whenever the program is executed under conditions of no electric discharge. If an illegal attempt is made to modify rate constants which are inaccessible to input, a warning diagnostic is issued and the illegal attempt is ignored unless declared to be fatal.

There are three subroutines which are synthesized by translation of the symbolic input reaction scheme into computer-coded equations:

---

**SUBROUTINE DNDT (N, T, NO, NDOT)**

---

This subroutine calculates the instantaneous rates of change of all of the dependent variables in the (first order) system of coupled differential equations (consisting of the master equation (4) and the circuit equations (93) or (94)). Miscellaneous optical (gain, absorption) and electrical parameters ( $e^-$ -beam voltage drop  $dV/dx$  and secondary  $e^-$  creation rate  $S_b$ , zero-energy  $e^-$  creation rate  $S_o$ ) are also obtained.

Input Parameters:

N           = Number of equations  
 T           = Independent variable, time (s)  
 NO(I)       = Vector of dependent variables: I = 1, NTYPE  
               are population densities ( $\text{cm}^{-3}$ ); NTYPE + 1 is  
               charge, q (Coul), and NTYPE + 2 is current, i (A)

Output Parameters:

NDOT       = Vector of rates of change of dependent variables:  
               NDOT(I) =  $d\text{NO}(I)/dt$ .



In addition to the formal calling parameters, there is also communication between DNDT and the main program LASER through labelled COMMON blocks. Since the integration subroutine GEAR is concerned only with the formal calling parameters shown, it need not be explicitly provided with miscellaneous experimental constants and input parameters available in the main program. Likewise, there are certain quantities which are useful by-products of the computations in DNDT such as SB ( $S_p$ ), SO ( $S_o$ ), DVDX ( $dv/dx$ ), and RATE(I) (the rates of Eq. (2)). Their inclusion in labelled COMMON is convenient for the direct communication of information to the main program LASER.

---

#### SUBROUTINE JACOB (N, T, NO, PHI)

---

This subroutine calculates a Jacobian required by the integration subroutine (GEAR). It computes the (instantaneous values) of the partial derivatives of the rates NDOT(I) with respect to the dependent variables NO(J) at time T. The calculation of the Jacobian is based upon exact expressions obtained from formal differentiation of the rate equations (4) and (93) (or (94)), rather than by numerical differencing. Its availability allows Subroutine GEAR to be utilized with a "method parameter" of MF = 1. Subroutine JACOB and DNDT share the same labelled COMMON blocks with the main program, although no computational results of JACOB are used by LASER itself. The input parameters for JACOB are the same as for DNDT described above.

#### Output Parameters:

PHI(I, J) = Jacobian array, dimensioned PHI(N, ...) in the calling program, defined by

$$PHI(I, J) = \partial NDOT(I) / \partial NO(J)$$

---

### SUBROUTINE LEVELS (N1, N2, NO)

---

This subroutine establishes the correspondence between the lower and upper levels of the inelastic electron collision processes, and the species of the molecular kinetics reaction scheme. It provides part of the linkage which couples the Boltzmann analysis to the molecular kinetics. Immediately prior to a call to Subroutine BOLTZ, this subroutine must be called to determine the (instantaneous) values of the lower and upper state population densities.

#### Input Parameters:

NO (I) = Vector of (instantaneous) population densities ( $\text{cm}^{-3}$ ) for the Ith species in the kinetic scheme.

#### Output Parameters:

N1 (I) = Vector of population densities for the lower states of the Ith inelastic electron collisions.

N2 (I) = Vector of population densities for the upper states of the Ith inelastic electron collisions.

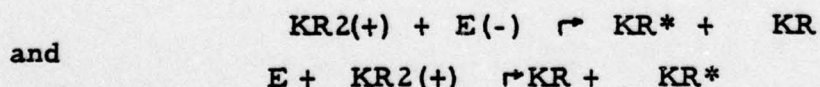
Sample output, obtained from synthesis of subroutines DNDT, JACOB, and LEVELS for the KrF laser system, will be presented later. The results of translation of the molecular kinetic scheme into computer-coded FORTRAN equations will be illustrated for several reactions. In addition to reaction translation, there is also generation of internal COMMENT card documentation, which makes the synthesized subroutines completely readable and understandable. They can be used as the source for creation of a BCD UPDATE program library, which can be catalogued and saved, if desired. If the reaction scheme is to be subsequently executed, the binary compilation should be saved.



## DATA BLOCK 2

The purpose of DATA BLOCK 2 is to provide updates or modifications to the electron cross section library, attached on TAPE8, immediately prior to execution. The updated file, generated on TAPE9, is then used for execution of the analysis and can be catalogued and saved for future access, if desired. Since the external electron cross section library can be originally constructed by "updating" an empty TAPE8 file with the totality of available data, the format for reading TAPE8, TAPE9, and DATA BLOCK 2 is identical.

DATA BLOCK 2, whose structure is shown in Table 3.2, consists of an arbitrary number of packages of electron cross section data for secondary electron collision processes. The first card of a package contains a 60-BCD character Hollerith field in which the symbolic reaction is specified. The syntax for reactions is quite flexible, and is the same as that described for DATA BLOCK 1 above. Embedded blanks are ignored, and the order of species is not important. Thus, when a search is made for cross section data for an electron collision process encountered in the molecular kinetic scheme, it is not required that the reaction be written identically as it occurs in the external electron data file. Only the content of two reactions compared must be identical; for example, the two reactions



would be recognized to be equivalent. An additional convention is used for specifying momentum transfer cross section for electron collisions with species X:



Table 3.2: DATA BLOCK 2  
(Cross Section Update)

---

Package 1	
Package 2	
⋮	
Package n:	

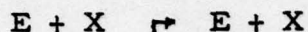
---

Card 1	KINETIC(6), UNITS, NPTS, MONTH (6A10, F7.3, I3, A10) This card contains a 60-BCD character field for the symbolic specification of an electron collision process. Cross section data entered on subsequent cards is assumed to be expressed in units of $\text{UNITS} \times 10^{-16} \text{ cm}^2$ . Default is UNITS = 1 if unspecified. NPTS defines subsequent data format.
Card 2	COMMENT(6) (6A10) 60-BCD character field for comment or data reference. This information is reproduced with requested tabular output of the cross section data, and is automatically extracted as the rate reference in a synthesis program.
Card 3	EV, vector of m electron energy values (eV),
Card 4	SIGMA, vector of m corresponding cross section data values. Format for Card 3, 4 is (mEn.0), where m = NPTS and n = 80/NPTS (truncate decimal residue).
⋮	⋮
Card i	Cf. description of Card 3,
Card i+1	Cf. description of Card 4,
⋮	⋮
Card 2k+1	Blank card terminates cross section data for the electron collision process of this package.

---

⋮	
---	--

---



Although momentum transfer cross sections must be included in the electron library file, the explicit inclusion of elastic or momentum transfer collisions in the molecular kinetic reaction scheme defined in DATA BLOCK 1 is not required.

The second parameter on the first card, UNITS, is a multiplicative factor to adjust the numerical cross section values, which are assumed to be entered in units of  $10^{-16} \text{ cm}^2$ . (If UNITS is not specified, it defaults to 1.0.) The third parameter, NPTS, specifies a variable FORMAT(mEn.0), where  $m = \text{NPTS}$  and  $n = 80/\text{NPTS}$  ( $n$  is an integer obtained from truncation of decimal residue). This FORMAT specifies the number of data fields on subsequent energy and cross section cards to be read from the current package. (If  $\text{NPTS} \leq 0$  or if  $\text{NPTS} > 10$ , program sets  $\text{NPTS} = 10$  by default.) The last parameter, MONTH, is a 10-BCD character specification of the date (e.g., 12/25/78) of cross section submission into the library file. If it is not provided, it is automatically generated by Subroutine UPDATE at the time it is added to the library.

The second card of a package contains a 60-BCD character field for comment or data reference. It is reproduced on requests for output plots or tables of cross sections, and is automatically extracted as the reference for TAPE4 data in the generation of a synthetic program.

Following the first two cards, there is an arbitrary number of card pairs  $i$  and  $i+1$ , ultimately terminated by a blank card, containing sequences of energies and corresponding cross section values. Card



i contains a sequence of energies (eV), which must be in monotonically ascending order, followed by card (i+1), which contains the corresponding cross section values (in units of  $\text{UNITS} \times 10^{-16} \text{ cm}^2$ ). The format specification is (mEn.0), as described above. For example, if NPTS = 8, the format would be (8E10.0), defining eight 10-column fields (into which F-numbers could be entered, if desired).

Ultimately, the collection of cross section packages must be terminated by an EOF card.

### DATA BLOCK 3

DATA BLOCK 3, shown in Fig. 3.3, consists of an arbitrarily long sequence of comment cards which will be reproduced in the output. It provides a convenient opportunity for documenting the output of an analysis with descriptive remarks. Format is (8A10).

### DATA BLOCK 4

DATA BLOCK 4, whose structure is shown in Fig. 3.4, defines experimental parameters, numerical control parameters, fatal error designation, data initialization, and output requests for execution of the synthesized analysis. It consists of six NAMELIST data groups, followed by an arbitrarily long sequence of cards which initialize the energies, molecular weights, and population densities of molecular species. The NAMELIST parameters are defined in Tables 3.5-3.10, which summarize the assumed units and default values. The NAMELIST groups have been constructed to have physically descriptive names, and to contain logically related variables.

The format for the sequence of species cards is (A10, 3E10.3, 10X, A10).



Table 3.3: DATA BLOCK 3  
(Descriptive Comments)

---

Card 1	COMMENT (8)	(8A10)
Card 2	COMMENT (8)	(8A10)
⋮	⋮	
Card n	COMMENT (8)	(8A10)
⋮	⋮	
EOF card termination.		

---

TABLE 3.4: DATA BLOCK 4  
(Execution Parameters)

1) \$CONTROL ... \$

Miscellaneous parameters related to numerical control of the calculations--convergence accuracy, integration order and method, electron energy resolution, interpolation order, fatal declaration of error conditions, frequency of output generation, etc. (Table 3.5).

2) \$PARAM ... \$

Pressure, temperature, and pulse length (Table 3.6).

3) \$OPTICAL ... \$

Optical cavity specifications--loss per pass or threshold coefficient, output coupling reflectivity, length, area, solid angle (Table 3.7).

4) \$EBEAM ... \$

External  $e^-$ -beam current density, energy, temporal and energy dependent characteristics (Table 3.8).

5) \$CIRCUIT ... \$

Capacitance, inductance, and resistance of external RLC driving circuit, initial charging voltage, discharge area and electrode separation (Table 3.9).

6) \$RATES ... \$

(Permissible) modifications to kinetic rate constants for the reaction scheme (Table 3.10).

The above NAMELIST cards are followed by (an arbitrary number of) cards for initialization of species parameters. These cards (which are ultimately terminated by an EOF card) are of the form:

NAME, P, E, MOLWT, OPTION (A10, 3E10.3, 10X, A10)

These cards define the energy E (eV) and molecular weight MOLWT (g/mole) of the species NAME. P is the concentration: if the total pressure is specified by the \$PARAM\$ card, the P values represent relative fractions. If the total pressure has not been previously specified, the values of P represent partial pressures (Torr), unless their values are  $> 1.0E\ 08$ , in which case they represent actual population densities ( $cm^{-3}$ ). (Cf. description of PTOT and ATM in Table 3.6.) If OPTION = 4HPLOT, a plot of NAME is generated.

TABLE 3.5: NAMELIST / CONTROL / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
EMAX	$u_{\max}$	eV	Electron energy range for solution of the Boltzmann equation is $[0, u_{\max}]$ . Default is EMAX = 20.0. During execution (if EXPAND = .TRUE.), the electron energy range is automatically expanded if certain convergence conditions were not met.
EXPAND			LOGICAL variable which instructs program to automatically expand the electron energy range $[0, u_{\max}]$ if the Boltzmann solution did not converge to relative accuracy EPS, or if the power discrepancy exceeds PCT. Default: EXPAND = .F.
MESH	MESH		Number of (equally spaced) intervals into which the electron energy range $[0, u_{\max}]$ is subdivided (cf. Eq. (73)). Default is MESH = MGRID. Program does not permit MESH MGRID.
PCT		%	Maximum permissible error in power balance for the electron kinetics analysis; if exceeded (and if EXPAND = .TRUE. was specified), program will attempt to attain better power balance by expanding the range $[0, u_{\max}]$ . Default: PCT = 5.0.
ITMAX			Maximum number of iterations permitted for the calculation of an electron distribution function $f_0(u)$ . If convergence to the required accuracy EPS was not attained, a diagnostic is generated, and program terminates unless EXPAND = .TRUE. Default is ITMAX = 100.



TABLE 3.5: NAMELIST /CONTROL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
TMAX		CP sec	Maximum CP time permitted for calculation of an electron distribution function (cf. description for ITMAX). Default is TMAX = 50.0.
EPS	$\epsilon$		Convergence parameter for solution of the Boltzmann equation (cf. Eq. (92)). Solution for the electron energy distribution proceeds by an iterative technique; as soon as the maximum relative change (over all discrete energies) between two successive iterations is $< \text{EPS}$ , convergence is declared. Default is EPS = .001.
TE	$T_e$	K	Initial electron temperature. Default is TE = TMOL.
IDEG			Degree of (polynomial) interpolation for defining the input electron cross section data over the uniform grid of MESH intervals. Default is IDEG = 2 (quadratic interpolation).
NCYCLE			The total specified pulse length, TPULSE, is subdivided into NCYCLE (equal) intervals of time $\Delta t = \text{TPULSE}/\text{NCYCLE}$ . At the discrete points $t_k = k\Delta t$ ( $k = 0, 1, \dots, \text{NCYCLE}$ ) the Boltzmann analysis is updated, and various output (as specified by the option vector IO) is generated. Default: NCYCLE = MAX; if NCYCLE > MAX, program sets NCYCLE = MAX.

TABLE 3.5: NAMELIST / CONTROL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
LIMIT			Number of complete time intervals over which the calculations are carried out. The total pulse length TPULSE is subdivided into NCYCLE (equal) intervals of time $\Delta t = \text{TPULSE} / \text{NCYCLE}$ , defining discrete times $t_k = k\Delta t$ ( $k = 0, 1, 2, \dots$ , NCYCLE). The calculations can be restricted to terminate at $k = \text{LIMIT}$ . Default is $\text{LIMIT} = \text{NCYCLE}$ . Program insures that $0 \leq \text{LIMIT} \leq \text{NCYCLE}$ .
MAXDER			The maximum derivative (order) used in the Gear integration technique. It must be less than eight for the Adams method, and seven for stiff methods. Default is $\text{MAXDER} = 7$ . (Cf. comments in Subroutine GEAR.)
METHOD			The specification of method in Subroutine GEAR. METHOD may be 0 (Adams predictor-corrector), 1 (multistep technique suitable for stiff systems), or 2 (same as case 1, except that partial derivatives are computed by numerical differencing). Default is $\text{METHOD} = 1$ (since both the rates $\dot{n}_i$ and the Jacobian $\partial \dot{n}_i / \partial n_i$ are provided by synthesized subroutines). Cf. discussion of Subroutine GEAR.
ETA			Error test for GEAR integration; the step size and order are adjusted to maintain this accuracy. Default; $\text{ETA} = .001$ . Cf. comments in Subroutine GEAR.



TABLE 3.5: NAMELIST / CONTROL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
FATAL(I)			<p>Vector of LOGICAL control parameters to specify that certain potential error conditions, if encountered, be treated as fatal: if condition I occurs, and FATAL(I) = .TRUE., execution of the analysis is terminated. (A diagnostic message is generated for each error condition.) Default is FATAL(I) = .FALSE. for conditions I = 1, 2, 3, ... 9; error 10 is automatically declared fatal and is inaccessible to input. Error conditions:</p> <ol style="list-style-type: none"> <li>1) Errors were detected in processing the input reaction scheme during subroutine synthesis. Modifications of the reaction scheme, corrections to the reaction syntax, changes in DIMENSION storage, or additions to the electron cross section file may be required. If FATAL(1) = .FALSE., the code ignores defective input.</li> <li>2) Unrecognized molecular species, which did not occur in the molecular kinetic reaction scheme, were encountered for initialization. If FATAL(2) = .FALSE., such species are assumed to be buffer gases and are included in the total pressure, and as constituents in the electron kinetics analysis (momentum transfer).</li> <li>3) Not all of the population densities for species present in the synthesized reaction scheme were initialized by input. If FATAL(3) = .FALSE., program initializes these population densities to zero, by default.</li> </ol>



TABLE 3.5: NAMELIST / CONTROL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
			<p>4) Not all of the energy levels were specified for the species present in the synthesized reaction scheme. If FATAL(4) = .FALSE., program sets them to zero by default.</p> <p>5) Errors were detected in the electron cross section data file (e.g., cross section not defined in the range <math>[0, u_{max}]</math>, cross section data not sequenced monotonically in energy, cross section data missing). Default: zero cross section.</p> <p>6) Mass, or momentum transfer cross section, for some of the gas species was zero. If FATAL(6) = .FALSE., momentum transfer for these gases is ignored in the electron kinetic calculations.</p> <p>7) An attempt was made to modify rate constants which the program considers to be inaccessible by input (e.g., the rate of a reverse process not originally present, a rate defined by detail balance, or a rate for a secondary electron excitation process in an electric discharge). Such an attempt is simply ignored if FATAL(7) = .FALSE.</p> <p>8) DIMENSION declarator constants read from TAPE4 (containing the data associated with the synthesized subroutines for a given reaction scheme) do not agree with those defined in the main program LASER. If new storage allocation is greater, there may be no problem. Caution is advised to insure that labeled COMMON blocks agree.</p>

TABLE 3.5: NAMELIST / CONTROL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
			9) Data on TAPE4 contained vectors which exceed maximum allocated DIMENSION storage in the main program, and must, therefore, be truncated upon input loading.
			10) Momentum transfer collision frequency was zero at some point in the electron energy range $[0, v_{\max}]$ . Since its inverse occurs in the Boltzmann equation, this condition is automatically declared fatal by the program.
IO(I)			Vector of integer constants for specification of output options $I, I = 1, 2, 3, \dots, 10$ . The total pulse duration TPULSE over which the analysis is integrated is subdivided into NCYCLE intervals that define discrete times $t_k = k \Delta t$ ( $\Delta t = \text{TPULSE} / \text{NCYCLE}$ , $k = 0, 1, 2, \dots, \text{LIMIT}$ ). At these discrete points, various output options can be requested. IO(I) represents (for $I = 1, 2, \dots, 7$ ) an integer multiple of the basic cycle index $k$ at which option I is to be generated (options 8, 9, and 10 occur only once, if $\text{IO} \neq 0$ ). Default is $\text{IO}(I) = 1$ ( $I = 1, 2, 3, \dots, 10$ ). The output specified by each IO parameter is the following:
1)			Tabular summary of plasma parameters ( $\bar{u}, T_e, D, \mu, \epsilon_k, \rho, \sigma, dn_e/dt, v_i, v_a$ , etc. Cf. Fig. 4.12.)
2)			Tabular summary of the electron distribution function $f_0(u)$ as a function of energy $u$ . (Cf. Fig. 4.13.)



TABLE 3.5: NAMELIST / CONTROL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
3)			Logarithmic plot of the normalized electron energy distribution $f_0(u)/f_0(0)$ as a function of energy $u$ (cf. Fig. 4.14)
4)			Logarithmic plot of $f_0(u)/f_B(u, T_e)$ , where $f_B(u, T_e)$ is the Boltzmann distribution for an effective temperature $T_e$ defined by $T_e = 2\bar{u}/3k$ (in terms of the average energy $\bar{u}$ of the actual distribution $f_0(u)$ ). (Cf. Fig. 4.15.)
5)			Tabular summary of electrical power partitioning and the forward and reverse excitation rates for all of the inelastic electron collisions included in the Boltzmann analysis. (Cf. Fig. 4.16.)
			Options 1-5 correspond to the output options OUT (5) for Subroutine BOLTZ.
6)			Tabular output of population densities and their rates of change (and effective instantaneous time constants) for all molecular species, and electrical and optical parameters. (Cf. Fig. 4.17.)
7)			Tabular summary of reaction sensitivities (cf. Fig. 4.18.)
8)			Tabular output of raw electron cross section data (cf. Fig. 4.10).
9)			Plots of electron cross section data (cf. Fig. 4.11).
10)			Table of reactions and modifications (if any) of rate constants (cf. Fig. 4.9).



TABLE 3.6: NAMELIST / PARAM / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
TPULSE		s	Normally, the total pulse length. TPULSE is subdivided into NCYCLE intervals of time over which the molecular kinetic and circuit equations are integrated. At the discrete times $t_k = k\Delta t$ ( $\Delta t = \text{TPULSE}/\text{NCYCLE}$ , $k = 0, 1, 2, \dots, \text{LIMIT}$ ), the Boltzmann equation is solved. The combination of NCYCLE, LIMIT, and TPULSE provides flexibility for the joint specification of total integration time and the frequency of electron kinetic updates.
TMOL	T	K	Molecular temperature. Default is TMOL = 300.0.
TE	$T_e$	K	Initial electron temperature. Default is TE = TMOL.
PTOT		Torr	Total pressure. Default is PTOT = 0.0.
ATM		atm	Total pressure. Default is ATM = 0.0.
There is a variety of alternative methods for specifying the pressure (or equivalently) the population densities of the species. If PTOT = 0.0, the program sets PTOT = 760. *ATM; then, if PTOT $\neq$ 0.0, input concentrations (to be entered by subsequent input) are assumed to be relative fractions, normalized to a total pressure PTOT. If PTOT = 0.0, it is assumed that input concentrations represent partial pressures (Torr), unless the values are $> 1.0\text{E } 08$ , in which case they represent actual population densities ( $\text{cm}^{-3}$ ).			

TABLE 3.7: NAMELIST /OPTICAL/ Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
LOSS	$\gamma$	%	Single pass loss for intracavity optical elements, exclusive of absorption in the gain medium. Default is LOSS = 0.0 (REAL).
REFLECT	R	%	A simple plane parallel cavity formed by a total reflector and an output coupling mirror of reflectivity R is assumed. The default is REFLECT = 0.0 (high cavity threshold results).
LENGTH	$L_g$	cm	Length of the active gain medium. If LENGTH $\leq$ 0.0 (REAL), default is LENGTH = 0.01.
CAVITY	$L_c$	cm	Length of the optical cavity (i.e., mirror separation). The default is CAVITY = LENGTH.
AREA	A	cm <sup>2</sup>	Area of the optical output aperture. Default is AREA = 0.0.
OMEGA	$\Omega$	sr	Solid angle subtended by the optical output aperture as viewed from the opposite end of the cavity. Default: OMEGA = $A/L_c^2$ . The buildup of the optical field occurs from amplification (by stimulated emission) of a fraction ( $\Omega/4\pi$ ) of the spontaneous noise. If OMEGA = 0.0, and if the initial value of NO(1) = 0.0, NO(1) will remain zero and there will be no contribution from the stimulated radiation processes in the kinetic scheme. (Cf. Eq. (12), (13), (122), and (123).)

TABLE 3.7: NAMELIST /OPTICAL / Parameters  
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
GAMMA	$\alpha_{th}$	$\text{cm}^{-1}$	Threshold loss coefficient. Default is GAMMA = 0.0. If GAMMA = 0.0, it is defined by Eq. (124), where $\gamma = \text{LOSS}$ and $L_g = \text{LENGTH}$ . If GAMMA $\neq$ 0.0 has been specified, the values of LOSS and REFLECT are ignored.



TABLE 3.8: NAMELIST /EBEAM / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
ENERGY		keV	Electron beam energy (for output reference only).
FACTOR			Multiplicative constant by which all $e^-$ -beam cross section values can be increased to account (in a qualitative way) for the larger energy deposition that results from multiple scattering effects in a high pressure gas. Default is FACTOR = 1.0.
UA, UB	$u_a, u_b$	eV	Cutoff energies to define the (normalized) electron source function $s(u)$ as a square wave (cf. Eq. (111)). Default is UA = UB = 0.0. If UB > EMAX, program sets UB = EMAX. If it were necessary, the program could easily be modified to provide a more complicated shape for $s(u)$ .
JB(21), TB(21)			Vectors to define the temporal shape of the $e^-$ -beam current density; program automatically renormalizes an input JB(I) to have a maximum value of JBEAM. JB(I) is assumed to be a function of the time TB(I), whose units are UNITS. Specification of JB, TB (which is optional) takes precedence over the alternative methods of defining temporal $e^-$ -beam current density described below. (The vector JB(I) is REAL.)
JBEAM	$J_e(\text{max})$	A/cm <sup>2</sup>	Maximum amplitude of $e^-$ -beam current density. Default is JBEAM = 0.0. (REAL variable)

TABLE 3.8: NAMELIST /EBEAM / Parameters  
(Continued)

FORTTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
UNITS			Units of time in which TB(I), TR, TF, TFALL, and TC times are expressed. Default is UNITS = 1.0E-09 (i. e. nanosecond).
TR	$t_r$		Rise time. Default is TR = 0.0.
TF	$t_f$		Fall time. Default is TF = 10,000.0.
TFALL	$t_F$		Fall time. Default is TFALL = 1.0.
TC	$t_c$		Cutoff time. Default is TC = 10,000.0.
<p>Unless the temporal shape of the e<sup>-</sup> beam current density has been explicitly specified in terms of the amplitude <math>J_b = JBEAM</math> and the numerical table [JB(I), TB(I)], it will be defined by</p> $J_b(t) = J_o \exp[-t/t_f] [1 - \exp(-t/t_r)], \quad 0 \leq t \leq t_c$ $J_b(t) = J_b(t_c) \exp[-(t - t_c)/t_F], \quad t_c < t,$ <p>where <math>J_o = JBEAM(t_r/t_f) [1 + t_f/t_r]^{(1 + t_r/t_f)}</math>, which automatically provides that the maximum amplitude of <math>J_b(t)</math> (which occurs at <math>t_o = t_r \ln[1 + t_f/t_r]</math>) shall be <math>J_b(\max) = JBEAM</math>.</p>			

TABLE 3.9: NAMELIST / CIRCUIT / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
KVOLT		kV	(REAL variable), giving the initial charging voltage across the capacitor in the external circuit. Default is KVOLT = 0.0.
RESIST	r		External circuit resistance. Default is RESIST = 0.0.
INDUCT	L	H	(REAL variable) representing the external circuit inductance. Default is INDUCT = 0.0.
CAPAC	C	F	External circuit capacitance. Default is CAPAC = 1.0.
AREA	A	cm <sup>2</sup>	Discharge electrode area. Default is AREA = 1.0.
DIST	d	cm	Discharge electrode separation. Default is DIST = 1.0.



TABLE 3.10: NAMELIST / RATES / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
KF(I), KR(I)	$k_f, k_r$		(REAL vectors) representing the forward and reverse rate constants for the Ith reaction in the kinetic scheme. (Units are $\text{cm}^2, \text{s}^{-1}, \text{cm}^3/\text{s}, \text{cm}^6/\text{s}, \dots$ , as appropriate.) This NAMELIST permits modification of the initial values of rate constants provided at the time of synthesis of the molecular kinetic sub-routines. Program considers some rate constants inaccessible to modification (e.g., rate constants for reverse reactions not originally present, rates related by detail balance, or secondary electron excitation rates in an electric discharge). The default values are the initial rates stored on the data TAPE4.

### 3.3 Description of Subroutines

The general laser kinetics program LASER requires 16 additional subroutines (in addition to the three which are synthesized, JACOB, DNDT, and LEVELS). An independent program, ELECT, has also been developed specifically for Boltzmann electron kinetics analysis and uses some of the same subroutines. Complete source deck listings for both main programs (LASER and ELECT), as well as for all subroutines used, are included in Vol. II of the present report. Fig. 3.11 summarizes the subroutines required for each program. In this section, some of the more important subroutines will be described. Program ELECT will be described in Sec. 3.4 below.

---

SUBROUTINE SYNTH(LTAPE, MTAPE, NTAPE, NSCRTCH, NDATA,  
NSIZE, MAXGAS, GAS, KMAX, NKMAX, LEV1, LEV2, DATE)

---

This subroutine translates the symbolic reactions of DATA BLOCK 1 into computer-coded equations for the synthesis of subroutines DNDT, JACOB, and LEVELS described in Sec. 3.2. It also compiles the data defining rate constants and references and the structure of the molecular kinetic reaction scheme to generate an associated file on unit NSCRTCH (= 4). Source code is generated as 80-BCD character records on unit MTAPE (= 3), which is compiled for execution. If future execution of a laser kinetics analysis based upon the input reaction scheme is anticipated, the data file on TAPE4 and the source code (and/or its binary compilation) should be catalogued and saved.

Input and output parameters for Subroutine SYNTH are summarized in Table 3.12. Specification of the record content of file NSCRTCH is most easily obtained directly from the listing.

Table 3.11: Deck Structure for Programs  
LASER and ELECT

Main Program --	LASER	ELECT
<u>Subroutines:</u>		
SYNTH	X	
GEAR	X	
ANALYZE	X	
SHAPE	X	
<u>Synthesized Subroutines:</u>		
JACOB	X	
DNDT	X	
LEVELS	X	
<u>Electron Kinetics Subroutines:</u>		
UPDATE	X	X
PLASMA	X	X
BOLTZ	X	X
<u>Utility Subroutines:</u>		
DECODE	X	X
SIMEQ	X	X
PLOT	X	X
AXIS	X	X
INTERP	X	X
SIMPSON	X	X
EDITOR	X	X
COVER	X	X
HEADINX	X	X



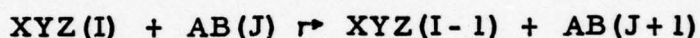
TABLE 3.12: Input Parameters for Subroutine SYNTH

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
LTAPE			File unit LTAPE is used for scratch purposes.
MTAPE, NTAPE			File units for synthesized FORTRAN source code generated. Subroutines DNDT and JACOB are synthesized simultaneously, on NTAPE and MTAPE respectively, as the reaction list of input DATA BLOCK 1 is processed. Subroutine LEVELS is then generated on NTAPE. Finally, NTAPE is copied on to MTAPE. At the termination of synthesis, MTAPE then contains three consecutive subroutines, JACOB, DNDT, and LEVELS.
NSCRTCH			File unit on which reaction data is written. TAPE NSCRTCH must be saved along with the FORTRAN source code if future execution of the synthetic program is anticipated.
NDATA			File unit containing the electron cross section library.
NSIZE			In the symbolic reaction scheme, the first NSIZE characters of a species name are recognized and all others ignored. $NSIZE \leq 10$ .
MAXGAS			Dimension declarator in calling program for maximum number of different species. Program automatically reserves 1 and 2 for radiation and secondary electrons, respectively.
KMAX			Dimension declarator in calling program for maximum number of reactions in the molecular kinetic scheme.

TABLE 3.12: Input Parameters for Subroutine SYNTH  
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
NKMAX			Dimension declarator in calling program for the maximum number of secondary electron collision processes in the mo- lecular kinetic reaction scheme.
GAS, LEV1, LEV2			Integer scratch arrays provided by the calling program for species names and identification of lower and upper excited states in electron collision processes.
DATE			(Integer) variable containing Hollerith specification of the date (e.g., 10H 10/17/78 ) of program generation.

The main purpose of Subroutine SYNTH is to dissect the syntax of (certain types of) symbolic reactions, and to translate the fundamental information content into computer-coded equations. It has been "taught" to recognize the meaning of a reasonably general class of expressions as well as to detect the occurrence of miscellaneous error conditions. If necessary, the user could extend its translation or error detection capabilities, and is at liberty to specify in detail the structure of the synthesized subroutines. For example, the present techniques could be extended in such a way that an encountered "species" such as "XYZ (I)" would be recognized as a representative member of a manifold of vibrational levels, and the reaction syntax,



could be interpreted to be a class of vibrational-vibrational exchange collisions to be translated into appropriate DO-LOOPS over I, J in the generated FORTRAN source code. The translation of reactions performed by the present version of SYNTH is best illustrated by examples and is therefore postponed until Sec. 4, where results for the KrF laser system are described.

---

SUBROUTINE GEAR (N, T, Y, SAVE, H, HMIN, HMAX, EPS, MF, YMAX, ERROR, KFLAG, JSTART, MAXDER, M, PW)

---

This subroutine was modified from "Subroutine DIFSUB", which appears in the work of Gear<sup>6</sup> on numerical initial value problems in ordinary differential equations. (Cf. Ref. 6, pp. 155-166.) It is a subroutine for integration of a "stiff" system of coupled, first order, differential equations with the capability for automatic control of the step size and order of predictor and corrector. The replacement of "MATINV" discussed in the "Note to Program" (cf. p. 158, Ref. 6)



has been implemented by the use of Subroutine SIMEQ to avoid the initial calculation of a matrix inverse, followed by successive pre-multiplications of a sequence of vectors with that inverse. Input and output parameters are completely described by COMMENT cards in the listing in Vol. II.

---

SUBROUTINE UPDATE (INFILE, NTAPE, NSCRTCH, LIST, DATE)

---

This subroutine searches two input data sources, a file unit INFILE and/or card input, to generate an updated electron cross section data library on unit NTAPE. (LASER uses INFILE = 8, NTAPE = 9.) The updated file on NTAPE contains all of the data of INFILE, modified with the additions or revisions defined by card input. A complete cross section data package (cf. Table 3.2 and the discussion of DATA BLOCK 2) must be provided for the initial addition, or subsequent modification, of any collision process. NSCRTCH is a scratch file. If LIST = .TRUE., the contents of the updated file NTAPE are generated in output. DATE is an (INTEGER) variable containing a 10-BCD Hollerith date (e.g. 10H 10/23/75 ).

---

SUBROUTINE PLASMA (NDATA, MAX, MESH, LHS, RHS, PROCESS, EV, F, G, Q, U0, UM, NTYPE, NAME, MISSING, ERROR, OUTSIDE, IDEG, OUT)

---

This subroutine scans the electron cross section library, on file unit NDATA, to extract the cross section data for input reaction defined by LHS and RHS, integer variables generated by Subroutine DEKODE which uniquely specify the left and right hand collision species. The reaction is also described by PROCESS (a 4-vector), containing a 40 BCD character (possibly abbreviated) symbolic expression of the re-

action (used for output purposes only). Input and output parameters are fully described in COMMENT cards in the listing.

---

```
SUBROUTINE BOLTZ (MAX, MESH, NK, GAS, FRACT, MIX, NMOL,
  TMOL, ITMAX, TMAX, EPS, KAPTION, DATE, OUT, EVCM, NE,
  PROCESS, U, N1, N2, NEL, S, SBEAM, SOURCE, X, XQ, QM, F,
  G, A, B, VSIG, POWER, PCOLL, DISCH, DEPOSIT, MU, D, EK,
  AMPS, UBAR, TE, CONVRGE, PBAL)
```

---

This subroutine implements the numerical solution of the Boltzmann equation for the electron energy distribution, using the computational algorithms described in detail in Sec. 2.3. Input parameters are described in Table 3.13, and output parameters in Table 3.14. Extensive internal COMMENT card documentation is also included in the listing, given in Vol. II.

---

```
SUBROUTINE DECODE (NAME, IMAGE, LHS, RHS, LABEL, GAS,
  NSIZE, NTYPE, LONG)
```

---

This subroutine dissects the symbolic reaction equations to determine the species on the left and right hand sides. A Hollerith specification of the reaction is provided as an input vector, IMAGE(I), I = 1, LONG. Embedded blanks are permitted, and up to NSIZE characters of a species name are recognized and the rest ignored (NSIZE  $\leq$  10). The vector NAME provided by the calling program contains the names of NTYPE species which have previously been encountered and stored; if additional new species are recognized in the reaction defined by IMAGE, the vector NAME is automatically extended to include them, and NTYPE is increased appropriately upon return. GAS(J,K) is an (INTEGER) array containing the (10 BCD character) Hollerith name of the Jth species (J = 1, 5) on the left (K = 1) and right (K = 2) side



TABLE 3.13: Input Parameters to Subroutine BOLTZ

FORTAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
MAX			DIMENSION declarator, defined for various vectors and arrays in the calling program (S, X, XQ, QM, F, G, A, B).
MESH	MESH		Number of (equal) subdivisions into which the electron energy interval $[0, u_{\max}]$ is partitioned (Eq. (73)). $MESH + 1 \leq MAX$
NK			Number of inelastic secondary electron collision processes included in the analysis (labeled by $\alpha$ in the sum of Eq. (41)).
GAS(K)			Names (containing up to 10 BCD characters) of the Kth gas in the mixture (declared INTEGER by calling program).
FRACT(K)			Relative fraction of the Kth gas in the mixture. BOLTZ automatically normalizes: $\sum_K FRACT(K) = 1.$
MIX			Number of gases in the mixture.  MIX, GAS(K), and FRACT(K) are communicated for output labeling only, and can be restricted, as desired, by the calling program (e. g., limited to the major constituents). The concentrations are automatically sorted into descending order.



TABLE 3.13: Input Parameters to Subroutine BOLTZ  
(Continued)

FORTAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
NMOL	N	cm <sup>-3</sup>	Total neutral particle density.
TMOL	T	K	Molecular temperature.
ITMAX			Maximum number of iterations permitted for attainment of convergence of electron energy distribution. If ITMAX ≤ 0, BOLTZ omits solution of Boltzmann equation, and transfers control directly to calculation of plasma parameters based upon the input distribution function F(I).
TMAX		CP sec	Maximum CP time allowed for calculation of the electron energy distribution function.
EPS	ε		Convergence parameter: maximum relative change (over all energies) of the electron distribution between two successive iterations (cf. Eq. (92)).
KAPTION			KAPTION(4) contains a 40 BCD character title for output captions.
DATE			INTEGER Variable, containing the date (e.g., 12/15/78).

TABLE 3.13: Input Parameters to Subroutine BOLTZ  
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
OUT(5)			LOGICAL vector of output requests: if OUT(I) = .TRUE., the following output is generated:
			1) Table of plasma parameters ( $\bar{u}$ , $T$ , $D$ , $\mu$ , $\epsilon_k$ , $v_d$ , $\rho$ , $\sigma$ , $dn_e/dt$ , $v_{mom}$ , $v_i$ , $v_a$ , etc. Cf. Figure 4.12.)
			2) Table of normalized electron distribution function $f_0(u)$ as a function of energy $u$ . (Cf. Fig. 4.13.)
			3) Plot of $f_0(u)/f_0(0)$ as a function of $u$ (cf. Fig. 4.14).
			4) (Logarithmic) plot of the relative distribution $f_0(u)/f_B(u)$ where $f_B(u)$ is the Maxwell distribution at the effective electron temperature $T_e$ defined for the actual distribu- tion $f_0(u)$ . (Cf. Fig. 4.15.)
			5) Table of secondary electron excitation rates, rates of el- ectron creation and loss, and power partitioning into all of the elastic and inelastic scattering mechanisms. Sum- mary of electrical power balance. (Cf. Fig. 4.16.)
EVCM	E	V/cm	Applied electric field.
NE	$n_e$	$cm^{-3}$	Secondary electron density.

TABLE 3.13: Input Parameters to Subroutine BOLTZ  
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
PROCESS			Array, dimensioned PROCESS(4,**) in the calling program, containing four words per column which provide a 40 BCD character specification of each of the inelastic collision processes (i.e., the symbolic reaction equation) for output.
U(J)	$u_{\alpha}$	eV	Vector containing the inelastic energy loss for the Jth electron collision process.
N1(J)	$N_{\alpha}$	$\text{cm}^{-3}$	Vector containing the neutral particle density of the initial state of the Jth inelastic electron collision process.
N2(J)	$N_{\alpha}^*$	$\text{cm}^{-3}$	Vector containing the neutral particle density of the final state of the Jth inelastic electron collision process.
NEL(J)			(Net) number of electrons (right hand side - left hand side) for the Jth electron collision process. (For reactions which conserve electrons, NEL = 0; for secondary ionization, NEL = 1; for attachment or recombination, NEL = -1, etc.)
S(I)	$s(u)$	$\text{eV}^{-1}$	Normalized $e^{-}$ -beam source function at energy $u_1 = (I-1)/\Delta u$ . (Cf. Eq. (106), (107), and (111).)
SBEAM	$S_b$	$\text{cm}^{-3} \text{s}^{-1}$	Total rate of creation by an external source of ionization (e.g. $e^{-}$ -beam) of electrons at positive energies ( $u > 0$ ).



TABLE 3.13: Input Parameters for Subroutine BOLTZ  
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
SOURCE	$S_o$	$\text{cm}^{-3} \text{s}^{-1}$	Total rate of creation of secondary electrons at zero energy from external reactions (i.e. excluding secondary ionization) Cf. Eq. (39), (68), and (109) for the definition of the external electron source function.
X(I)	$u_i$	eV	Vector of electron energies, $X(I) = (I - 1)\Delta u$ (cf. Eq. (73)).
XQ(I, J)		$\text{eVcm}^2$	Array of quantities, dimensioned XQ(MAX, **) in the calling program, defined by $XQ(I, J) = X(I)Q_J(I)$ , where $Q_J(I)$ is the Jth inelastic cross section at energy $X(I)$ .
QM(I, K)		eVcm $\text{eV}^2/\text{cm}$	Array (containing two column vectors) dimensioned QM(MAX, 2) in the calling program, defined by $QM(I, 1) = u_i^+ / \langle N Q_m(u_i^+) \rangle,$ $QM(I, 2) = (u_i^+)^2 \langle (2m/M) N Q_m(u_i^+) \rangle,$ <p>where <math>u_i^+ = u_i + \Delta u/2</math> (Cf. Eq. (32), (75), (77), and (78).)</p>
G, A, B			Scratch vectors, dimensioned G(MAX), A(MAX, 3), and B(MAX) in the calling program (Cf. OUTPUT description).

TABLE 3.13: Input Parameters to Subroutine BOLTZ  
(Continued)

FORTAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
F(I)	$f_i$	$\text{eV}^{-3/2}$	$F(I) = f_i = f(u_i)$ is, upon input, an initial guess vector (dimensioned $F_{\text{MAX}}$ ) in the calling program) for the electron energy distribution (which need not be normalized) defined over the energy grid $X(I)$ . Numerical solution of the Boltzmann equation proceeds by an iterative scheme initiated with the input guess; if $ITMAX \leq 0$ , plasma parameters can be calculated for the specified input vector $F(I)$ .

TABLE 3.14: Output Parameters for Subroutine BOLTZ

FORTAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
VSIG	$\langle vQ_{\pm\alpha} \rangle$	$\text{cm}^3/\text{s}$	Array, dimensioned $VSIG(2, **)$ in the calling program, containing the forward and reverse electron excitation rates for the inelastic collision processes: (Cf. Eq. (49).)  $VSIG(1, J) = \langle vQ_{+J}(u) \rangle$ , $VSIG(2, J) = \langle vQ_{-J}(u) \rangle$ , Jth collision process

TABLE 3.14: Output Parameters for Subroutine BOLTZ  
(Continued)

FORTTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
POWER(J)	$P_{\alpha}$	$\text{W/cm}^3$ or $\text{W/elect}$	(Net) power density partitioned into the Jth inelastic process (accounting for forward and reverse collisions, as required). If $\text{NEL} = 0$ , $P_{\alpha} = n_e e u_{\alpha} [N_{\alpha} \langle v Q_{\alpha}(u) \rangle - N_{\alpha}^* \langle v Q_{-\alpha}(u) \rangle].$ <p>If <math>\text{NEL} &gt; 0</math>, the term with <math>N_{\alpha}^*</math> does not appear; if <math>\text{NEL} &lt; 0</math>, the appropriate expression is</p> $P_{\alpha} = n_e e (2e/m)^{1/2} N_{\alpha} \int_0^{\infty} du u^2 f_0(u) Q_{\alpha}(u).$ <p>(Cf. Eq. (61), (62), (67), and accompanying discussion.) If <math>n_e = 0</math>, plasma parameters are all independent of electron density, and calculation is assumed to be per electron (i.e. units of <math>W/\text{electron}</math>).</p>
PCOLL	$\sum_{\alpha} P_{\alpha}$	$\text{W/cm}^3$ or $\text{W/elect}$	Total electrical power density partitioned into inelastic scat- tering processes: $\text{PCOLL} = \sum_J \text{POWER}(J)$



TABLE 3.14: Output Parameters for Subroutine BOLTZ  
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
ELASTIC	$P_e$	$W/cm^3$ or $W/elect$	Electrical power density converted to elastic heating of the molecular gas: $P_e = en_e (2e/m)^{1/2} \int_0^{\infty} du u^2 < (2m/M)NQ_m > [f_0 + \frac{kT}{e} \frac{df_0}{du}]$ (Cf. Eq.(67).) If $n_e = 0$ , subroutine calculates $P_e/n_e$ (power per electron).
DEDT		$W/cm^3$ or $W/elect$	Rate of change of energy density of stored electron kinetic energy: $DEDT = e \bar{u} dn_e / dt$
DISCH		$W/cm^3$ or $W/elect$	Electrical power density into the gas from the electric discharge: $DISCH = en_e \mu E^2$
DEPOSIT		$W/cm^3$ or $W/elect$	Power density deposited as electron kinetic energy by external source of ionization: (Cf. Eq. (67), (71), and (110).) $DEPOSIT = e < U^+ > S_b$

TABLE 3.14: Output Parameters for Subroutine BOLTZ  
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
<p>The units for all of the power density terms described above are <math>W/cm^3</math> if the input value NE is not zero. If <math>n_e = 0</math>, the calculations correspond to setting <math>n_e = 1</math> (i.e. parameters are calculated per electron), and corresponding units become <math>W/electron</math>.</p>			
DNEDT	$dn_e/dt$	$cm^{-3}s^{-1}$	Self-consistently calculated value of the rate of change of the secondary electron density (Cf. Eq. (56) and accompanying discussion.) Upon input, DNEDT can be entered as an initial estimate of $dn_e/dt$ , which is then determined self-consistently in an iterative loop.
DLNEDT	$dn_e/dt/n_e$	$s^{-1}$	Logarithmic derivative of electron density: $DLNEDT = d/dt(\ln n_e) = dn_e/dt/n_e$
IONIZE	$\nu_i$	$s^{-1}$	Total secondary ionization frequency.
ATTACH	$\nu_a$	$s^{-1}$	Attachment (and recombination) frequency.
VD	$v_d$	$cm/s$	Drift velocity: $v_d = \mu E$ (Cf. Eq. (50) and (55).)
MU	$\mu$	$cm^2/Vs$	Electron mobility (cf. Eq. (50)).

TABLE3.14: Output Parameters for Subroutine BOLTZ  
(Continued)

FORTAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
EK	$\epsilon_k$	eV	Characteristic energy (cf. Eq. (54)).
AMPS	$J/n_e$	Acm	Electric discharge current density, per unit electron density: $AMPS = J/n_e = ev_d$
UBAR	$\bar{u}$	eV	Average electron energy (cf. Eq. (52)).
TE	$T_e$	K	Effective electron temperature: $\bar{u} = (3/2)kT_e$ (Eq. (53)).
CONVRGE			LOGICAL variable defining (if .TRUE.) successful convergence of the iterative solution to the Boltzmann equation (41).
PBAL		%	If the Boltzmann equation is correctly solved, the equation (67) for power balance will be satisfied, except for a possible discrepancy $\Delta P$ resulting from numerical errors: $PBAL = 100 \Delta P / (DISCH + DEPOSIT)$ .
F, G, B	$f_i$	$eV^{-3/2}$	Upon successful convergence, $F(I)$ is the normalized electron distribution; $G(I) = F(I)/F(1) = f_o(u)/f_o(0)$ ; and $B(I) = f_o(u)/f_B(u, T_e)$ , where $f_B(u, T_e)$ is the Boltzmann distribution at the effective temperature $T_e$ .



of the reaction, and LABEL(J, K) are the integer labels for GAS(J,K) which correspond to the sequential ordering of the species in the vector NAME(I), I = 1, NTYPE. If there are less than the five species permitted on the left (or right) hand side, the default value for arrays GAS and LABEL are 1H (blank) and 0, respectively. Further details concerning reaction syntax were given in the discussion of DATA BLOCK 1 above.

In order to make possible a simple comparison between two sequences of collision partners (which may be only rearranged), Subroutine DEKODE also generates INTEGER variables LHS and RHS to uniquely describe the left and right hand side of the reaction. If a sequence of collision partners contains species defined by the integer indices  $l_J$ , two sums are defined

$$L = \sum_J l_J,$$

$$LSQ = \sum_J l_J^2.$$

L and LSQ are then encoded into an (INTEGER) variable, with format (I4,I6), to define an "identifier" (i.e., LHS or RHS), which is invariant to a permutation of the component species  $l_J$  and believed to be unique, for all practical purposes. The identifiers LHS and RHS are used as Hollerith variables, and contain numbers with no physical significance.

LASER initializes the vector NAME(I) in such a way that I = 1 and 2 are reserved for radiation and secondary electrons, respectively.

### Miscellaneous Utility Subroutines

---

#### SUBROUTINE SIMEQ (A, M, N, N1, SING)

---

The purpose of this subroutine is to solve an  $N \times N$  system of simultaneous equations of the form

$$\sum_J A(I, J) X(J) = B(I),$$

where  $I = 1, 2, 3, \dots, N$ . Input consists of putting the  $N \times N$  matrix of coefficients into the upper left hand box of the array A, which is dimensioned A(M,NCOL) in the calling program. N1 different B-vectors can be specified, stored in successive columns to the right of the  $N \times N$  matrix (cf. Fig. 3.2). ( $M \geq N$ , and  $N+N1 \leq \text{NCOL}$ .) Upon output, the coefficients in the upper left hand  $N \times N$  box are destroyed, and the solution vectors X replace the corresponding input vectors B. That is, the N1 column vectors B of length N form an  $N \times N1$  array B, which is transformed to  $A^{-1}B$  upon output. In particular, if N B-vectors are chosen to form the unit matrix, output will consist of the inverse  $A^{-1}$ . SING is a logical variable which is returned .FALSE. unless the coefficient matrix is singular.

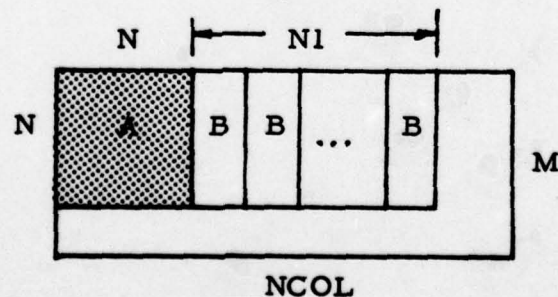


Fig. 3.2: Input array structure for SIMEQ.

---

SUBROUTINE PLOT (MM, MP, MULT, Y, Y0, DY, X, X0, DX,  
SCALEX, SCALEY, SAME, CLEAR, CENTER, NAME, NP, IP)

---

This subroutine generates linear, logarithmic, or semilogarithmic plots for NP vectors ( $NP \leq 10$ ),  $Y(I, J)$ ,  $J = 1, 2, \dots, NP$ . A variety of options exist for automatic scaling of the X- and Y-axes to convenient (integer) tick mark divisions, for simultaneous or independent scaling of data, and for output labeling. Extensive documentation, definition of input parameters, and instructions for usage can be found in the COMMENT cards in the listing.

---

SUBROUTINE AXIS (SCALE, XMAX, XMIN, X0, DX, XDC)

---

This subroutine is used for automatic scaling of axes for Subroutine PLOT. XMAX and XMIN are input values of the maximum and minimum values of the vector to be scaled. The range of values (XMAX - XMIN) is to be spanned by a convenient origin X0 and integer tick-mark spacing DX. XDC is set equal to zero unless the range  $10 DX < X0/1000$ , in which case XDC is set equal to X0, X0 is reset to zero, and XMAX and XMIN are reduced by an amount XDC. Thus, XDC corresponds to a "dc baseline" that is returned nonzero whenever the range of the plot is very small relative to the absolute magnitude of the values themselves.

---

SUBROUTINE INTERP (IDEG, XP, YP, X, Y, MULT, N)

---

This subroutine will interpolate a vector  $Y(I)$ , assumed to be a function of a vector  $X(I)$ , to produce that value YP which corresponds to



the value XP. IDEG = 1, 2, 3, ... specifies linear, quadratic, ... interpolation. The vectors X(I) and Y(I) provided by the calling program are sampled with a repetition index MULT, with N points defined at I = 1, (1+MULT), ... (1+(N-1)MULT) used. (Normal usage is MULT = 1.) Values of X(I) must be in ascending order. XP need not lie within the range of the vector X(I), but if it falls outside, linear interpolation is automatically used.

---

SUBROUTINE SIMPSON (F, M, H, ANS)

---

This subroutine integrates (Simpson method) a function defined as a vector F over N = 2M subintervals of width H, with result ANS.

---

SUBROUTINE EDITOR (INPUT, LIST)

---

This subroutine reads 80-BCD character records on unit INPUT to an EOF and rewrites them onto TAPE5, creating an effective card input file on TAPE5 each time a data block is processed. LIST = .TRUE. produces an output "playback" listing of the input card images, thus providing an exact output record of the input card decks.

---

SUBROUTINE COVER (TITLE, NPAGE)

---

NPAGE identical cover pages, each containing a three-line block-lettered title defined by TITLE(3), are generated for output.

---

SUBROUTINE HEADINX (JSYMB, JPAGE, MESSAGE)

---

This subroutine converts a 10-character phrase defined by an input vector MESSAGE(10) to block-letters. Refer to listing for usage.

### 3.4 Boltzmann Analysis Program

An independent program (ELECT) has been developed, concurrently with LASER, for Boltzmann analysis of a specified gas mixture and (sequence of) E/N values. As Table 3.11 shows, these two programs share the same subroutine file for those computational tasks which are common to both. Furthermore, the structure of the external electron cross section library is compatible for use with either program (cf. description of DATA BLOCK 2 in Sec. 3.2). A complete listing of ELECT, documented by COMMENT cards, is given in Vol. II.

Input deck structure for execution of the analysis consists of a set of data blocks, each terminated by an EOF (7/8/9 card), as shown in Fig. 3.3. The first data block is identical to DATA BLOCK 2 (for an update of the electron cross sections) described in Sec. 3.2. The second, DATA BLOCK A, consists of an (optional) sequence of symbolic reactions (60 BCD characters) to specify a set of secondary electron collisions to which the Boltzmann kinetics analysis will be restricted. If none are specified, the program will automatically use the available electron cross section library and retain all collision processes which involve any of the species which are subsequently initialized. DATA BLOCK A is followed by an arbitrary number of data blocks containing physical parameters for execution. The syntax for DATA BLOCK A is the same as that described previously for the reactions in DATA BLOCK 1 and DATA BLOCK 2.

The structure of DATA BLOCK B containing execution parameters is shown in Table 3.15. NAMELIST entry with suitable default initialization is used for input of numerical control parameters, physical data, and initialization of the components of the mixture.

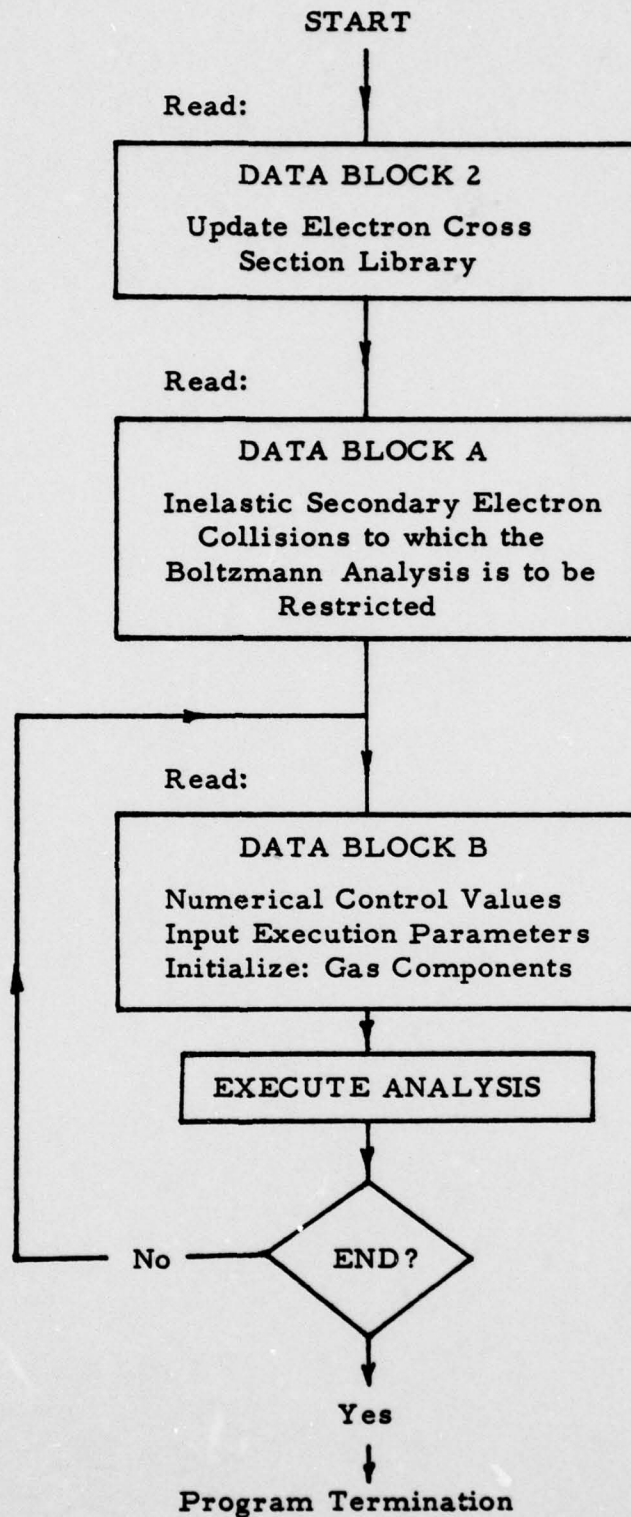


Fig. 3.3: Input data deck structure for Program ELECT.



TABLE 3.15: DATA BLOCK B  
(Boltzmann Execution Parameters)

---

1) \$CONTROL ... \$

Miscellaneous parameters related to numerical control of the calculations--convergence accuracy, energy resolution, interpolation order, output options, etc.

2) \$PARAM ... \$

Pressure, temperature, and E/N values

3) \$SOURCE ... \$

Parameters related to the magnitudes ( $S_o$  and  $S_p$ ) and energy dependence of an external ionization source function (e.g.,  $e^-$ -beam).

4) Arbitrarily long package of species cards for specification of concentrations, energies, and molecular weights

-----

1) NAME, P, E, MOLWT (A10,3E10.3)

2) NAME, P, E, MOLWT

:

i) NAME, P, E, MOLWT

:

-----

These cards define the energy E (eV), molecular weight MOLWT (g/mole), and concentration P of the species NAME. If the total pressure has been specified by the \$PARAM ... \$ entry, the P values represent partial fractions; if not, they represent partial pressures (Torr) unless their values are  $> 1.0E\ 08$ , in which case they represent actual population densities ( $cm^{-3}$ ).

---

### 3.5 Execution Control Cards

In the present section, some illustrative examples of the typical control card sequences required for execution of Program LASER and ELECT will be given. Obviously, job control language is characterized by considerable variations between different computer systems, as well as by fairly rapid evolutionary changes for any given system. Since the present programs were developed for execution under Extended Fortran Compilation on the CDC 6000 and CYBER Series of computers, the control card syntax appropriate for that system will be illustrated.

First of all, it is convenient to create, from the FORTRAN source deck, a BCD UPDATE program library for convenience in modifying the program if necessary. Fig. 3.4a illustrates the creation of such a file, which is given the name "LASERBCD" and catalogued and saved for future access. Furthermore, the binary compilation file has been catalogued and saved as "LASERFTN" for future execution of the code. A similar sequence of operations for Program ELECT is shown in Fig. 3.4b.

Assuming that the user finds the present version of the source code satisfactory, it can be used for synthesis and execution of analysis with the control cards and deck structure shown in Fig. 3.5. The input reaction scheme specified in DATA BLOCK 1 is translated into FORTRAN subroutines on TAPE3, which is subsequently used as the source for creation of a BCD UPDATE program library that is catalogued and saved with the name "KRFB CD". The file of data associated with the reaction scheme (created on TAPE4) is catalogued and saved with the name "KRFDATA". Two binary compilation files are

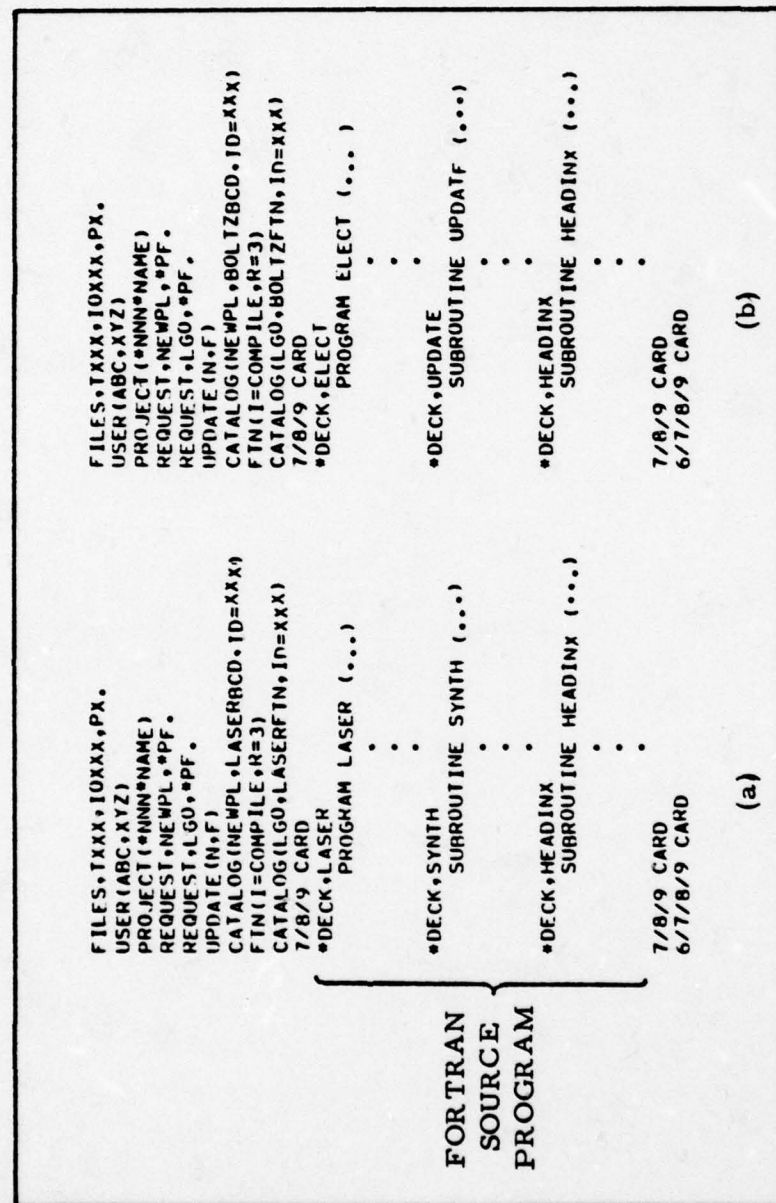


Fig. 3.4: Creation of a BCD UPDATE program library from the FORTRAN source deck, and a binary compilation file for program execution.





created. The compilation of the synthesized subroutines (i.e. JACOB, DNDT, and LEVELS) for the input reaction scheme is catalogued as "KRFBIN". The complete binary file (containing the main program LASER, all of its subroutines, and the subroutines just synthesized) is catalogued as "KRFLASER". The analysis which follows (defined by DATA BLOCK 2, 3, 4) is then executed under the binary file KRF-LASER. Note that no electron cross section library has been attached on TAPE8; the first time the program is run, DATA BLOCK 2 must contain card input of all available electron cross section data for the initial creation of such a library on TAPE9, which is shown catalogued as CROSSECTIONS. For all future execution of an analysis based upon the input reaction scheme, the binary file KRFLASER can be used, and CROSSECTIONS can be attached to TAPE8, as shown in Fig. 3.6.

If it is desired to modify the present version of the program, this can easily be done using UPDATE procedures. If these modifications include (but are not necessarily limited to) changes in subroutine SYNTH, the control cards and deck structure shown in Fig. 3.7 are appropriate. The three previously created permanent files LASERBCD, LASERFTN, and CROSSECTIONS are attached as designated. Modified subroutines are compiled and the old versions replaced by the new using the COPYL command. The new binary compilation file is catalogued (as LASERFTN) and the old one purged. Program LASER is then executed in its updated version, according to the input of DATA BLOCK 1, 2, 3, and 4. Revisions or additions to the electron cross section data of DATA BLOCK 2 are incorporated permanently by cataloging the updated file on TAPE9 as "CROSSECTIONS" and purging the initial file that was attached to TAPE8. If modifications to program LASER do not involve subroutine SYNTH, and it is only desired to make cer-

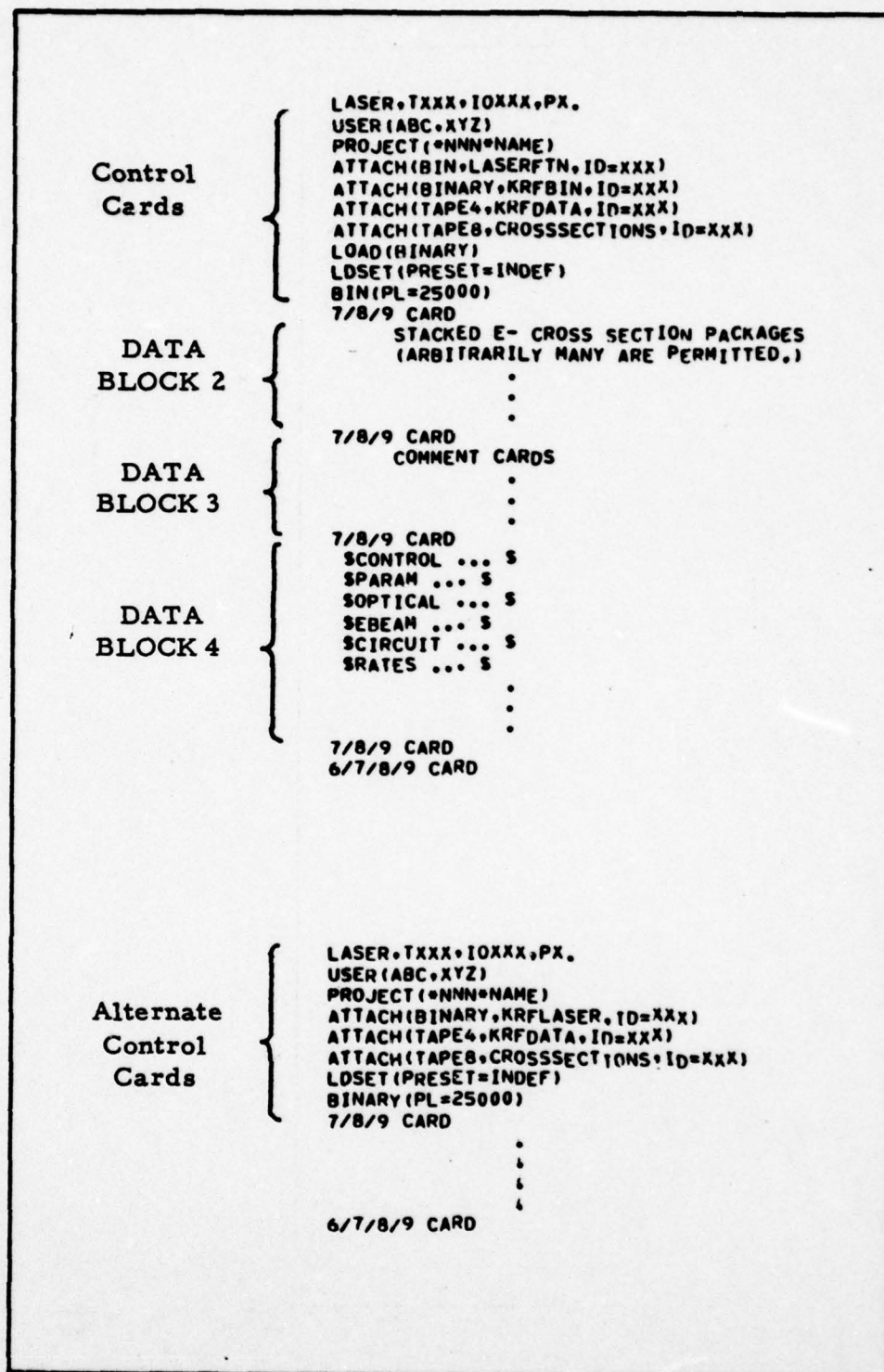


Fig. 3.6: Execution of the analysis by loading LASERFTN and KRFBIN, or the complete binary file KRFLASER.



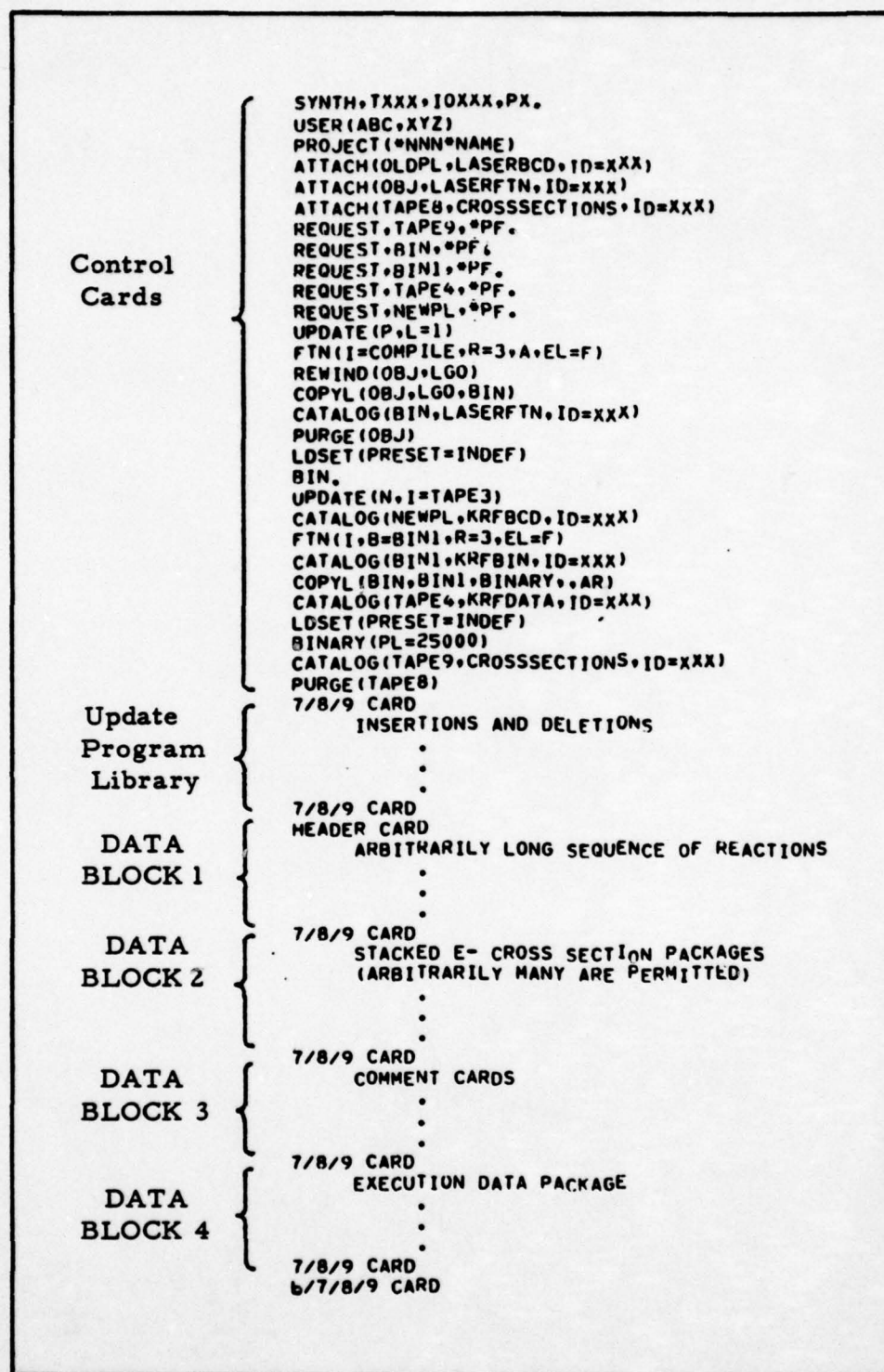


Fig. 3.7: Synthesis and catalog of program KRFBCD under a modified version of LASERBCD, followed by execution of the analysis.

tain changes related to execution of the analysis (not involving the synthesis of subroutines), Fig. 3.8 contains the appropriate control card and input deck structure.

It is conceivable that the user may desire to make changes both in the main program LASER (or in any of its subroutines) and in the synthetic subroutines (JACOB, DNNDT, or LEVELS). To facilitate this, it is convenient to have catalogued the BCD UPDATE program library KRFBCD (as described in Fig. 3.5). Both LASERBCD and KRFBCD can be updated, with their modified subroutines replaced (by COPYL) on the binary compilation file KRFLASER used for execution. It would be much more difficult to extend the translation capabilities of subroutine SYNTH to automatically recognize new reaction syntax, or to incorporate new computational features into the molecular kinetic subroutines, than it would be to merely modify the synthetic subroutines generated by the present program. There are, therefore, situations where an update of the program library KRFBCD (supplemented by any changes required for insuring compatibility with LASER or its subroutines) would probably be more efficient than an attempt to extend subroutine SYNTH. On the other hand, extensions which are likely to be of general applicability to future usage of the code should probably be incorporated directly into subroutine SYNTH.

Execution of the Boltzmann analysis program ELECT can be carried out with the control card sequence and data deck structure shown in Fig. 3.9. The electron cross section data library CROSSSECTIONS (discussed above) is compatible with either program (LASER, ELECT) and the structure of the electron update input (DATA BLOCK 2) is identical for both programs. Obviously, the same procedures for program modification by update of BOLTZBCD (as discussed for LASERBCD) are possible.

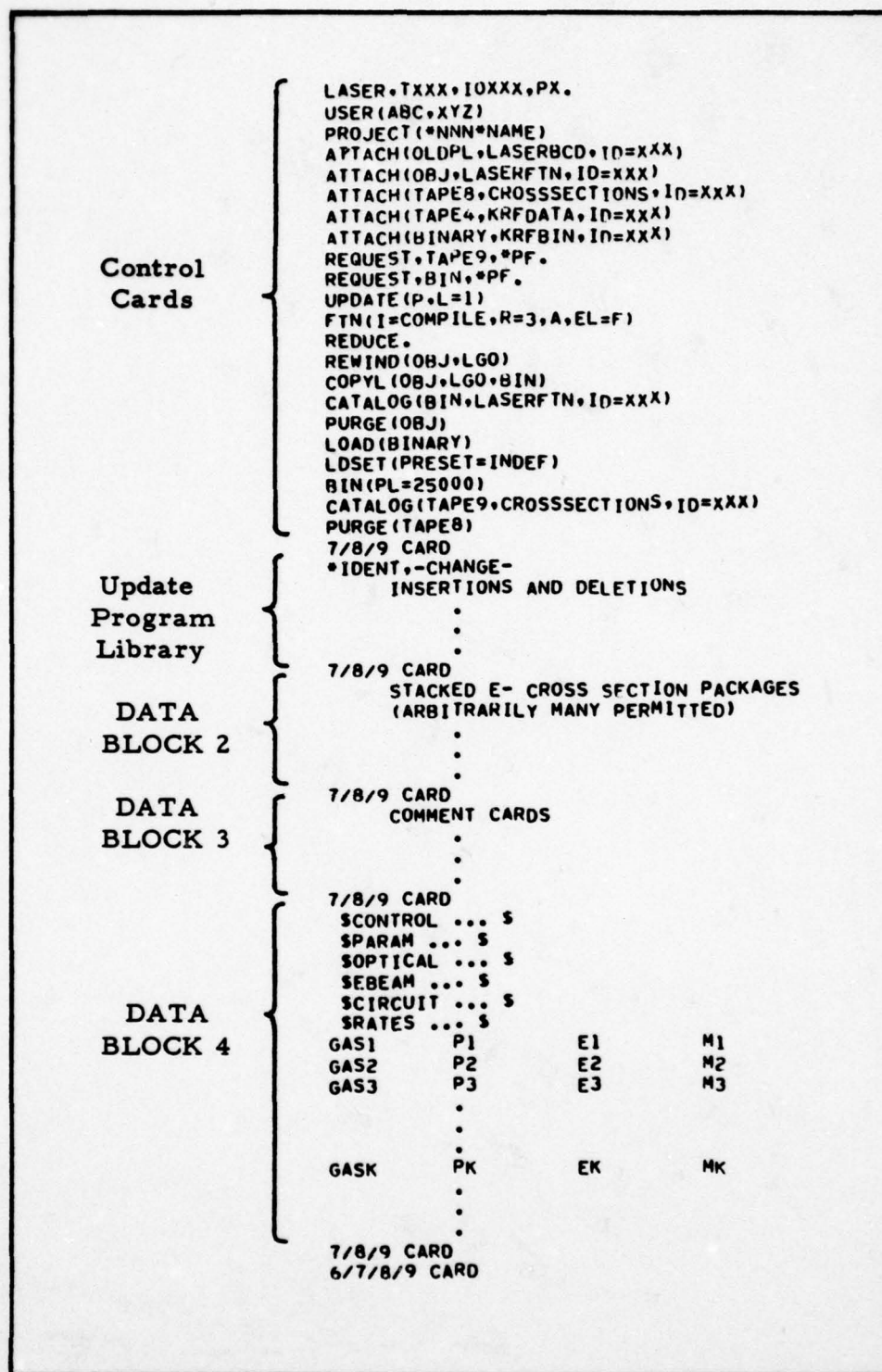


Fig. 3.8: Program library LASERBCD is modified by update, previous binary file KRFBIN is loaded, and analysis is executed under new version of LASERFTN.



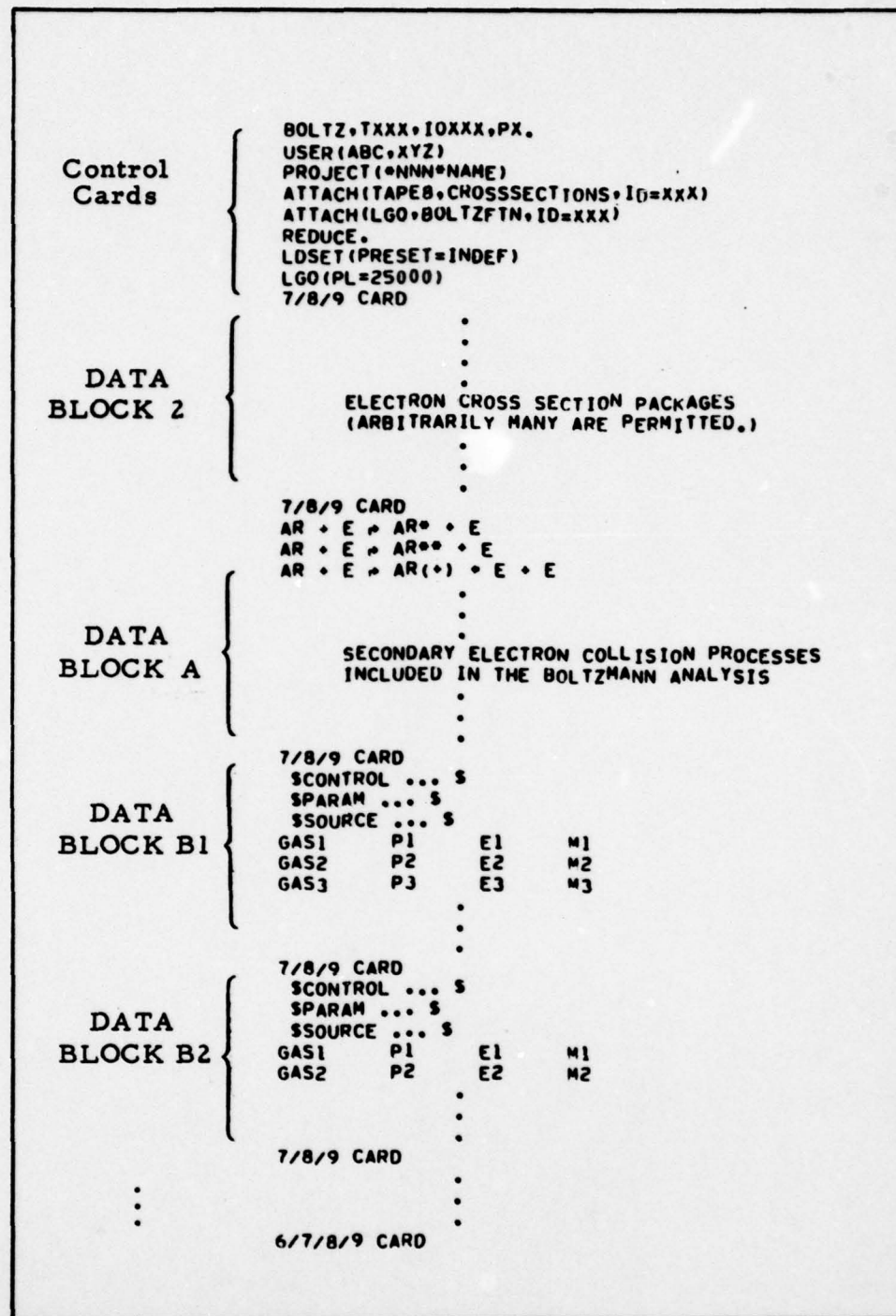


Fig. 3.9: Execution of the Boltzmann program ELECT.

#### 4.0 KrF LASER KINETICS: Illustrative Example of Program Synthesis and Execution

The Computer Program LASER that was described in Sec. 3 can be used to (automatically) synthesize and execute (for a reasonably arbitrary reaction scheme) a coupled analysis of molecular kinetics, electron kinetics, radiative extraction, and external (RLC) driving circuit. In this section, usage of the code will be illustrated with sample output obtained from analysis of the KrF laser kinetic system<sup>1-5</sup>. Names of permanent files in the discussion of control cards in Sec. 3.5 were chosen in anticipation of this example.

##### 4.1 Molecular Kinetic Subroutine Generation

As many as 80 reactions have been proposed as being of possible importance for the KrF laser kinetic reaction scheme. Fig. 4.1 shows the "playback" (generated in output by subroutine EDITOR) of the exact input card images of DATA BLOCK 1 (used in the deck structure of Fig. 3.5, for example) for synthesis of a KrF laser kinetics analysis. The header Card 1 contains three (10 BCD character) computer words ("NORTHROP ", "KRF LASER ", and "KINETICS ") which name the generated program and are used for a three-line block-letter title in subsequent output. Following the header card, there are 80 pairs of cards which define the kinetic reaction scheme and its rate constants (cf. description of DATA BLOCK 1 in Sec. 3.2).

The reactions of Fig. 4.1 are processed by Subroutine SYNTH and are translated into FORTRAN subroutines (JACOB, DNDDT, and LEVELS). During the translation process, Subroutine SYNTH also generates its own COMMENT card documentation of the synthesized subroutines in

CARD NO. 1 2 3 4 5 6 7 8  
12345678901234567890123456789012345678901234567890

1	....	NORTHROP KRF LASER KINETICS
2	....AR + E	AR + E
3	....	
4	....KR + E	KR + E
5	....	
6	....AR + E	AR + E
7	....	
8	....KR + E	KR + E
9	....	
10	....AR + E	AR + E
11	....	
12	....KR + E	KR + E
13	....	
14	....AR + E	AR + E
15	....	
16	....KR + E	KR + E
17	....	
18	....AR + E	AR + E
19	....	
20	....KR + E	KR + E
21	....	
22	....AR + E	AR + E
23	....	
24	....KR + E	KR + E
25	....	
26	....AR2(+) + E	AR + AR
27	....	
28	....KR2(+) + E	KR + KR
29	....	
30	....F2 + E	F + F
31	....	
32	....AR2 + E	AR + AR + E
33	....	
34	....1.00 E-07	KR + KR + E
35	....	
36	....1.00 E-07	
37	....AR + HE	AR(+) + HE + E
38	....	
39	....4.34 E-18	
40	....AR + HE	AR + HE
41	....	
42	....1.24 E-18	1.24 E-18
43	....	
44	....KR + HE	KR(+) + HE + E
45	....	
46	....	
47	....	
48	....	
49	....	
50	....	
51	....	
52	....	
53	....	
54	....	
55	....	
56	....	
57	....	
58	....	
59	....	
60	....	
61	....	
62	....	
63	....	
64	....	
65	....	
66	....	
67	....	
68	....	
69	....	
70	....	
71	....	
72	....	
73	....	
74	....	
75	....	
76	....	
77	....	
78	....	
79	....	
80	....	
81	....	
82	....	
83	....	
84	....	
85	....	
86	....	
87	....	
88	....	
89	....	
90	....	
91	....	
92	....	
93	....	
94	....	
95	....	
96	....	
97	....	
98	....	
99	....	
100	....	

[illegible]

**Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme.**





CARD NO. 1 2 3 4 5 6 7 8  
12345678901234567890123456789012345678901234567890

[illegible]

12345678901234567890123456789012345678901234567890

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme.  
(Continued)

CARD NO. 1 2 3 4 5 6 7 8  
1234567890123456789012345678901234567890

121	....	1.00 E-09		SRI REPORT NO.	MP 76-99,	DEC., 1976
122	....	ARKRF* * KR	* KR2F* * AR			
123	....	1.00 E-10		SRI REPORT NO.	MP 76-99,	DEC., 1976
124	....	KRF* * F2	* KR * F * F2			
125	....	1.00 E-09		SRI REPORT NO.	MP 76-99,	DEC., 1976
126	....	ANF* * F2	* AR * F * F2			
127	....	1.00 E-09		SRI REPORT NO.	MP 76-99,	DEC., 1976
128	....	AR2F* * KR	* KRF* * AR * AR			
129	....	1.0E-10				
130	....	AR* * M *	AR* * M			
131	....	1.00 E-10				
132	....	KR* * M *	KR* * M			
133	....	1.00 E-10				
134	....	ARF* * AR * F		SRI REPORT NO.	MP 76-99,	DEC., 1976
135	....	3.30 E 07		SRI REPORT NO.	MP 76-99,	DEC., 1976
136	....	AR2* * AR *	AR			
137	....	3.80 E 06		SRI REPORT NO.	MP 76-99,	DEC., 1976
138	....	ARKR* * AR * KR				
139	....	3.0E+06				
140	....	KR2* * KR * KR				
141	....	3.30 E 06		SRI REPORT NO.	MP 76-99,	DEC., 1976
142	....	AR2F* * AR * AR * F		SRI REPORT NO.	MP 76-99,	DEC., 1976
143	....	2.00 E 08		SRI REPORT NO.	MP 76-99,	DEC., 1976
144	....	ARKRF* * AR * KR * F		SRI REPORT NO.	MP 76-99,	DEC., 1976
145	....	5.00 E 07		SRI REPORT NO.	MP 76-99,	DEC., 1976
146	....	KR2F* * KR * KR * F		SRI REPORT NO.	MP 76-99,	DEC., 1976
147	....	6.70 E 07				
148	....	KRF* * KR * F * HNU		R. BURNHAM, S. S. SEARLES (SUBMITTED TO JCP)		
149	....	1.10 E 08		LASER TRANSITION! STIMULATED EMISSION X-SECTION		
150	....	KRF* * RAD	* KR * F * RAD			
151	....	2.00 E-16				
152	....	F2 * RAD * F * F				
153	....	1.50 E-20		A. MANDEL, PHYS REV A3, 251 (1971)		
154	....	f * RAD * f * E		CROSS SECTION UNKNOWN		
155	....	5.40 E-18				
156	....	KR2F* * RAD	* AR* * KR * F			
157	....	1.00 E-99				
158	....	AR2(+) * RAD	* AR * AR (+)	STEVENS (PARK CITY CONFERENCE)		
159	....	1.50 E-17				
160	....	KR2(+) * RAD	* KR * KR (+)			

[illegible]

**Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme.**  
(Continued)



SUMMARY OF CARD IMAGES FOR INPUT DATA DECK  
(DATE: 01/04/79)

CARD NO.	1	2	3	4	5	6	7	8
	123456789012345678901234567890123456789012345678901234567890							
161 ... 3.50 E-18			J. WEST (NRIC)					
	1	2	3	4	5	6	7	8
	123456789012345678901234567890123456789012345678901234567890							

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme.  
(Continued)

order to make them completely readable and accessible to modification. Fig. 4.2, 4.3, and 4.4 present samples of the FORTRAN statements generated for subroutines DNDT, JACOB, and LEVELS, respectively. Although it would be impractical to reproduce the entire listings of these synthesized subroutines here, it is informative to present excerpts which illustrate the translation for miscellaneous representative types of collisions, as is done in Fig. 4.2 and 4.3.

As the reaction queue of DATA BLOCK 1 is scanned by Subroutine SYNTH, input reference data, informative comments, and/or warning diagnostics are generated to produce an output summary, shown in Fig. 4.5. A reaction with unacceptable syntax or content is ignored, although processing continues. (An ignored reaction is not assigned a number in the summary of Fig. 4.5.) After the entire reaction list has been processed, a cross-reference table, illustrated by Fig. 4.6, is generated. This table provides for rapid identification of all reactions that involve any particular species, and is convenient whenever it is desired to delete some species from the kinetic scheme.

After generation of the FORTRAN source code on TAPE3 and construction of the data file on TAPE4, there is an exit from program LASER. TAPE3 is used as the source for creation of a BCD UPDATE file (cf. Fig. 3.5) which is catalogued as KRFBCD, and its binary compilation is combined with LASERFTN to create file KRFLASER for execution. The data file on TAPE4 is catalogued as KRFDATA.

#### 4.2 Execution of the Analysis

With the use of permanent files KRFDATA and KRFLASER, the analysis can be executed, either as a continuation from the initial synthesis

C	SUBROUTINE DNDT (N, T, NO, NDOT)	DNDT	2
C	.....	DNDT	3
C		DNDT	4
C		DNDT	5
C	THIS SUBROUTINE WAS SYNTHESIZED BY EDITING AN INPUT FILE OF SYM-	DNDT	6
C	BOLIC REACTIONS WHICH DEFINE A COUPLED SYSTEM OF ELECTRON AND	DNDT	7
C	MOLECULAR KINETICS. IT RETURNS THE RATES NDOT(I) = (D/DT)NO(I),	DNDT	8
C	I = 1,2,...,NTYPE (CM-3/SEC). RATE CONSTANTS KF AND KR HAVE UNITS	DNDT	9
C	OF CM2, SEC-1, CM3/SEC, CM6/SEC, ... AS APPROPRIATE.	DNDT	10
C		DNDT	11
C	THE GENERAL KINETICS SYNTHESIS PROGRAM WHICH AUTOMATICALLY GEN-	DNDT	12
C	ERATED THIS SUBROUTINE WAS DEVELOPED BY --	DNDT	13
C		DNDT	14
C	-----	DNDT	15
C	I	DNDT	16
C	I DR. WILLIAM B. LACINA	DNDT	17
C	I NORTHROP RESEARCH AND TECHNOLOGY	DNDT	18
C	I ONE RESEARCH PARK	DNDT	19
C	I PALOS VERDES PENINSULA, CA 90274	DNDT	20
C	I TEL: (213) 377-4811, EXT. 322	DNDT	21
C	I	DNDT	22
C	-----	DNDT	23
C		DNDT	24
C	.....	DNDT	25
C		DNDT	26
C	DIMENSION NO(1), NDOT(1)	DNDT	27
C	REAL NO, NTOT, NDOT, NOISE, NE, KF, KR, KB, KT, MU, L0, IBEAM,	DNDT	28
C	1 JBEAM, LENGTH	DNDT	29
C		DNDT	30
C	COMMON / DATA / RATE( 200), KF( 200), KR( 200), VSIG(2, 25), E(30)	DNDT	31
C	COMMON / CONST / NTOT, TMOL, FREQ, HNU	DNDT	32
C	COMMON / DISCH / L0, C0, R0, MU, AREA, D	DNDT	33
C	COMMON / SOURCE / UPLUS, JBEAM, DVDX, DEPOSIT, ENERGY, SB, S0	DNDT	34
C	COMMON / GAINS / ALPHA, GAMMA, GAIN, ABSORB, OMEGA, LENGTH, CAVITY	DNDT	35
C		DNDT	36
C	DATA KB, E0, H, C, P1 / 8.614E-05, 1.602E-19, 6.625E-34,	DNDT	37
C	1 3.000E+10, 3.14159 /	DNDT	38
C		DNDT	39
C	IBEAM = JBEAM*DEPOSIT*SHAPE(T)	DNDT	40
C	KT = KB*TMOL	DNDT	41
C	DO 1 I = 1,N	DNDT	42
C	1 NDOT(I) = 0.	DNDT	43
C	NDOT(I) = - C*GAMMA*NO(I)	DNDT	44
C	ALPHA = GAIN = HNU = FREQ = NOISE = DVDX = 0.	DNDT	45
C	SB = S0 = 0.0	DNDT	46
C		DNDT	47
C	GAIN = SIGMA*(N2-N1) IS THE LASER TRANSITION GAIN	DNDT	48
C	ABSORB = SUMK(SIGMA(K)*NK) IS THE TOTAL ABSORPTION OF THE MEDIUM	DNDT	49
C	ALPHA = (GAIN-ABSORB) IS THE NET GAIN IN THE MEDIUM	DNDT	50
C	GAMMA = THRESHHOLD GAIN COEFFICIENT (CM-1)	DNDT	51
C		DNDT	52
C	CAVITY = MIRROR SEPARATION (CM)	DNDT	53
C	LENGTH = LENGTH OF ACTIVE MEDIUM (CM)	DNDT	54
C	OMEGA = AREA/CAVITY**2	DNDT	55
C	AREA = AREA OF OPTICS (CM2)	DNDT	56
C	GAMMA = (LOSS + LN(1/R)/2)/LENGTH	DNDT	57
C		DNDT	58

Fig. 4.2: (Synthesized) Subroutine DNDT listing.



C	.....	DNDT	59
C		DNDT	60
C	THE FOLLOWING REACTIONS DEFINE THE KINETICS --	DNDT	61
C		DNDT	62
C	1 AR + E → AR* + E	DNDT	63
C		DNDT	64
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	65
C	KF( 1) = VSIG(1, 1)	DNDT	66
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	67
C	KR( 1) = VSIG(2, 1)	DNDT	68
C		DNDT	69
C	R = KF(1)*NO(3)*NO(2) - KR(1)*NO(4)*NO(2)	DNDT	70
C		DNDT	71
C	RATE( 1) = R	DNDT	72
C	NDOT(3) = NDOT(3) - R	DNDT	73
C	NDOT(4) = NDOT(4) + R	DNDT	74
C		DNDT	75
C	2 KR + E → KR* + E	DNDT	76
C		DNDT	77
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	78
C	KF( 2) = VSIG(1, 2)	DNDT	79
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	80
C	KR( 2) = VSIG(2, 2)	DNDT	81
C		DNDT	82
C	R = KF(2)*NO(5)*NO(2) - KR(2)*NO(6)*NO(2)	DNDT	83
C		DNDT	84
C	RATE( 2) = R	DNDT	85
C	NDOT(5) = NDOT(5) - R	DNDT	86
C	NDOT(6) = NDOT(6) + R	DNDT	87
C		DNDT	88
C	3 AR + E → AR** + E	DNDT	89
C		DNDT	90
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	91
C	KF( 3) = VSIG(1, 3)	DNDT	92
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	93
C	KR( 3) = VSIG(2, 3)	DNDT	94
C		DNDT	95
C	R = KF(3)*NO(3)*NO(2) - KR(3)*NO(7)*NO(2)	DNDT	96
C		DNDT	97
C	RATE( 3) = R	DNDT	98
C	NDOT(3) = NDOT(3) - R	DNDT	99
C	NDOT(7) = NDOT(7) + R	DNDT	100
C		DNDT	101
C	4 KR + E → KR** + E	DNDT	102
C		DNDT	103
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	104
C	KF( 4) = VSIG(1, 4)	DNDT	105
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	106
C	KR( 4) = VSIG(2, 4)	DNDT	107
C		DNDT	108
C	R = KF(4)*NO(5)*NO(2) - KR(4)*NO(8)*NO(2)	DNDT	109
C		DNDT	110
C	RATE( 4) = R	DNDT	111
C	NDOT(5) = NDOT(5) - R	DNDT	112
C	NDOT(8) = NDOT(8) + R	DNDT	113
C		DNDT	114
C	5 AR* + E → AR** + E	DNDT	115

Fig. 4.2 (Continued)

C			DNDT	140
C	7	AR + E → AR(+) + E + E	DNDT	141
C			DNDT	142
C		FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	143
C		KF( 7) = VSIG(1, 7)	DNDT	144
C			DNDT	145
C		R = KF(7)*NO(3)*NO(2)	DNDT	146
C			DNDT	147
C		RATE( 7) = R	DNDT	148
C		NDOT(2) = NDOT(2) + R	DNDT	149
C		NDOT(3) = NDOT(3) - R	DNDT	150
C		NDOT(9) = NDOT(9) + R	DNDT	151
C			DNDT	152
C				
C	13	AR2(+) + E → AR* + AR	DNDT	212
C			DNDT	213
C		FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	DNDT	214
C		KF( 13) = VSIG(1,13)	DNDT	215
C			DNDT	216
C		R = KF(13)*NO(11)*NO(2)	DNDT	217
C			DNDT	218
C		RATE( 13) = R	DNDT	219
C		NDOT(2) = NDOT(2) - R	DNDT	220
C		NDOT(3) = NDOT(3) + R	DNDT	221
C		NDOT(4) = NDOT(4) + R	DNDT	222
C		NDOT(11) = NDOT(11) - R	DNDT	223
C			DNDT	224
C			DNDT	225
C				
C	16	AR2* + E → AR + AR + E	DNDT	251
C			DNDT	252
C			DNDT	253
C		R = KF(16)*NO(16)*NO(2)	DNDT	254
C			DNDT	255
C		RATE( 16) = R	DNDT	256
C		NDOT(3) = NDOT(3) + R + R	DNDT	257
C		NDOT(16) = NDOT(16) - R	DNDT	258
C			DNDT	259
C				
C	19	AR + HE- → AR* + HE-	DNDT	288
C			DNDT	289
C		E1 = + E( 3)	DNDT	290
C		E2 = + E( 4)	DNDT	291
C		R = KF(19)*NO(3) - KR(19)*NO(4)	DNDT	292
C		S = R	DNDT	293
C		R = R*IBeam/E0	DNDT	294
C			DNDT	295
C		RATE( 19) = R	DNDT	296
C		NDOT(3) = NDOT(3) - R	DNDT	297
C		NDOT(4) = NDOT(4) + R	DNDT	298
C		U = (E2 - E1)	DNDT	299
C			DNDT	300
C		E-BEAM ENERGY DEPOSITION --	DNDT	301
C		DVdX = DVdX + U*S	DNDT	302
C			DNDT	303
C			DNDT	304

Fig. 4.2 (Continued)

C 20	KR = HE- * KR(*) + HE- * E	DNDT	305
C		DNDT	306
	E1 = * E( 5)	DNDT	307
	E2 = * E(10) + E( 2)	DNDT	308
	R = KF(20)*NO(5)	DNDT	309
	S = R	DNDT	310
	R = R*IBEAM/E0	DNDT	311
C		DNDT	312
	RATE( 20) = R	DNDT	313
	NDOT(2) = NDOT(2) + R	DNDT	314
	NDOT(5) = NDOT(5) - R	DNDT	315
	NDOT(10) = NDOT(10) + R	DNDT	316
	U = (E2 - E1)	DNDT	317
C		DNDT	318
C	SECONDARY ELECTRON CREATION--	DNDT	319
	SB = SB + R	DNDT	320
	U = U + UPLUS	DNDT	321
C		DNDT	322
C	E-BEAM ENERGY DEPOSITION --	DNDT	323
	DVOX = DVOX + U*S	DNDT	324
C		DNDT	325
C		DNDT	359
C 24	KH(*) + KR + M * KR2(*) + M	DNDT	360
C		DNDT	361
	R = KF(24)*NO(10)*NO(5)*NTOT	DNDT	362
C		DNDT	363
	RATE( 24) = R	DNDT	364
	NDOT(5) = NDOT(5) - R	DNDT	365
	NDOT(10) = NDOT(10) - R	DNDT	366
	NDOT(12) = NDOT(12) + R	DNDT	367
C		DNDT	368
C		DNDT	377
C 26	AR(*) + KR * AR + KR(*)	DNDT	378
C		DNDT	379
C	REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --	DNDT	380
C		DNDT	381
	E1 = * E( 9) + E( 5)	DNDT	382
	E2 = * E( 3) + E(10)	DNDT	383
	KR( 26) = KF( 26)*EXP(-(E1-E2)/KT)	DNDT	384
C		DNDT	385
	R = KF(26)*NO(9)*NO(5) - KR(26)*NO(3)*NO(10)	DNDT	386
C		DNDT	387
	RATE( 26) = R	DNDT	388
	NDOT(3) = NDOT(3) + R	DNDT	389
	NDOT(5) = NDOT(5) - R	DNDT	390
	NDOT(9) = NDOT(9) - R	DNDT	391
	NDOT(10) = NDOT(10) + R	DNDT	392
C		DNDT	393
C		DNDT	658
C 50	AR2* + AR2* * AR2(*) + AR + AR + E	DNDT	659
C		DNDT	660
	R = KF(50)*NO(16)*NO(16)	DNDT	661
C		DNDT	662
	RATE( 50) = R	DNDT	663
	NDOT(2) = NDOT(2) + R	DNDT	664
	NDOT(3) = NDOT(3) + R + R	DNDT	665
	NDOT(11) = NDOT(11) + R	DNDT	666
	NDOT(16) = NDOT(16) - R - R	DNDT	667
C		DNDT	668
C	CREATION OF (ZERO ENERGY) SECONDARY ELECTRONS--	DNDT	669
C		DNDT	670
	S0 = S0 + R	DNDT	671
C		DNDT	672

Fig. 4.2 (Continued)



C			DNDT	865
C	66	$KR^* \leftarrow M \leftarrow KR^* \leftarrow M$	DNDT	866
C			DNDT	867
C		REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --	DNDT	868
C			DNDT	869
		$E1 = \cdot E(8)$	DNDT	870
		$E2 = \cdot E(6)$	DNDT	871
		$KR(66) = KF(66) * EXP(-(E1-E2)/KT)$	DNDT	872
C			DNDT	873
		$R = KF(66) * NO(8) * NTOT - KR(66) * NO(6) * NTOT$	DNDT	874
C			DNDT	875
		$RATE(66) = R$	DNDT	876
		$NDOT(6) = NDOT(6) + R$	DNDT	877
		$NDOT(8) = NDOT(8) - R$	DNDT	878
C			DNDT	879
C	67	$ARF^* \leftarrow AR \leftarrow F$	DNDT	880
C			DNDT	881
		$R = KF(67) * NO(20)$	DNDT	882
C			DNDT	883
		$RATE(67) = R$	DNDT	884
		$NDOT(3) = NDOT(3) + R$	DNDT	885
		$NDOT(14) = NDOT(14) + R$	DNDT	886
		$NDOT(20) = NDOT(20) - R$	DNDT	887
C			DNDT	888
C			DNDT	941
C	74	$KRF^* \leftarrow KR \leftarrow F \leftarrow HNU$	DNDT	942
C			DNDT	943
		$R = KF(74) * NO(22)$	DNDT	944
C			DNDT	945
		$RATE(74) = R$	DNDT	946
		$NDOT(5) = NDOT(5) + R$	DNDT	947
		$NDOT(14) = NDOT(14) + R$	DNDT	948
		$NDOT(22) = NDOT(22) - R$	DNDT	949
C			DNDT	950
C		PHOTON NUMBER DENSITY INCREASED BY NOISE --	DNDT	951
C			DNDT	952
		$NOISE = NOISE + R * OMEGA / 4. / PI$	DNDT	953
C			DNDT	954
C	75	$KRF^* \leftarrow RAD \leftarrow KR \leftarrow F \leftarrow RAD$	DNDT	955
C			DNDT	956
C		(STIMULATED EMISSION PROCESS, WITH $NO(1) = INTEN/C/HNU$ )	DNDT	957
C			DNDT	958
		$E1 = \cdot E(22) + E(1)$	DNDT	959
		$E2 = \cdot E(5) + E(14) + E(1)$	DNDT	960
		$HNU = E0 * (E1 - E2)$	DNDT	961
		$FREQ = HNU/H$	DNDT	962
C			DNDT	963
		$R = KF(75) * NO(22) * NO(1)$	DNDT	964
		$R = R * C$	DNDT	965
C			DNDT	966
		$RATE(75) = R$	DNDT	967
		$NDOT(1) = NDOT(1) + R$	DNDT	968
		$NDOT(5) = NDOT(5) + R$	DNDT	969
		$NDOT(14) = NDOT(14) + R$	DNDT	970

Fig. 4.2 (Continued)

```

      NDOT(22) = NDOT(22) - R
C
      R = KF(75)*NO(22)
      GAIN = GAIN + R
      ALPHA = ALPHA + R
C
C 76 F2 + RAD + F + F
C
C      (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(76)*NO(13)*NO(1)
      R = R*C
C
      RATE( 76) = R
      NDOT(1) = NDOT(1) - R
      NDOT(13) = NDOT(13) - R
      NDOT(14) = NDOT(14) + R + R
C
      R = KF(76)*NO(13)
      ALPHA = ALPHA - R
C
C 77 F- + RAD + F + E
C
C      (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(77)*NO(15)*NO(1)
      R = R*C
C
      RATE( 77) = R
      NDOT(1) = NDOT(1) - R
      NDOT(2) = NDOT(2) + R
      NDOT(14) = NDOT(14) + R
      NDOT(15) = NDOT(15) - R
C
C      CREATION OF (ZERO ENERGY) SECONDARY ELECTRONS--
C
      S0 = S0 + R
C
      R = KF(77)*NO(15)
      ALPHA = ALPHA - R
C
C 78 KR2F+ + RAD + AR+ + KR + F
C
C      (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(78)*NO(23)*NO(1)
      R = R*C
C
      RATE( 78) = R
      NDOT(1) = NDOT(1) - R
      NDOT(4) = NDOT(4) + R
      NDOT(5) = NDOT(5) + R
      NDOT(14) = NDOT(14) + R
      NDOT(23) = NDOT(23) - R
C
      R = KF(78)*NO(23)
      ALPHA = ALPHA - R

```

```

DNDT  971
DNDT  972
DNDT  973
DNDT  974
DNDT  975
DNDT  976
DNDT  977
DNDT  978
DNDT  979
DNDT  980
DNDT  981
DNDT  982
DNDT  983
DNDT  984
DNDT  985
DNDT  986
DNDT  987
DNDT  988
DNDT  989
DNDT  990
DNDT  991
DNDT  992
DNDT  993
DNDT  994
DNDT  995
DNDT  996
DNDT  997
DNDT  998
DNDT  999
DNDT 1000
DNDT 1001
DNDT 1002
DNDT 1003
DNDT 1004
DNDT 1005
DNDT 1006
DNDT 1007
DNDT 1008
DNDT 1009
DNDT 1010
DNDT 1011
DNDT 1012
DNDT 1013
DNDT 1014
DNDT 1015
DNDT 1016
DNDT 1017
DNDT 1018
DNDT 1019
DNDT 1020
DNDT 1021
DNDT 1022
DNDT 1023
DNDT 1024
DNDT 1025
DNDT 1026
DNDT 1027

```

Fig. 4.2 (Continued)

165



C	SUBROUTINE JACOB (N, T, NO, PHI)	JACOB	2
C	.....	JACOB	3
C		JACOB	4
C	THIS SUBROUTINE WAS SYNTHESIZED BY EDITING AN INPUT FILE OF SYM-	JACOB	5
C	BOLIC REACTIONS WHICH DEFINE A COUPLED SYSTEM OF ELECTRON AND	JACOB	6
C	MOLECULAR KINETICS EQUATIONS. IT RETURNS THE JACOBIAN MATRIX,	JACOB	7
C		JACOB	8
C	PHI(I,J) = D[NDOT(I)]/D[NO(J)]	JACOB	9
C		JACOB	10
C	WHERE I,J = 1,2,3,...NTYPE. N IS THE DIMENSION DECLARATOR FOR PHI	JACOB	11
C	IN THE CALLING PROGRAM. THE RATE CONSTANTS KF AND KR HAVE UNITS	JACOB	12
C	OF CM2, SEC-1, CM3/SEC, CM6/SEC, ... AS APPROPRIATE.	JACOB	13
C		JACOB	14
C	THE GENERAL KINETICS SYNTHESIS PROGRAM WHICH AUTOMATICALLY GEN-	JACOB	15
C	ERATED THIS SUBROUTINE WAS DEVELOPED BY --	JACOB	16
C		JACOB	17
C	-----	JACOB	18
C	I	JACOB	19
C	I DR. WILLIAM B. LACINA	JACOB	20
C	I NORTHROP RESEARCH AND TECHNOLOGY	JACOB	21
C	I ONE RESEARCH PARK	JACOB	22
C	I PALOS VERDES PENINSULA, CA 90274	JACOB	23
C	I TEL: (213) 377-4811, EXT. 322	JACOB	24
C	I	JACOB	25
C	-----	JACOB	26
C		JACOB	27
C	.....	JACOB	28
C		JACOB	29
C	DIMENSION PHI(N,1), NO(1)	JACOB	30
C	REAL NO, NTOT, NDOT, NOISE, NE, KF, KR, KB, KT, MU, L0, IBEAM,	JACOB	31
C	1 JBEAM, LENGTH	JACOB	32
C		JACOB	33
C	COMMON / DATA / RATE( 200), KF( 200), KR( 200), VSIG(2, 25), E(30)	JACOB	34
C	COMMON / CONST / NTOT, TMOL, FREQ, HNU	JACOB	35
C	COMMON / DISCH / L0, C0, R0, MU, AREA, D	JACOB	36
C	COMMON / SOURCE / UPLUS, JBEAM, DVDX, DEPOSIT, ENERGY, SB, S0	JACOB	37
C	COMMON / GAINS / ALPHA, GAMMA, GAIN, ABSORB, OMEGA, LENGTH, CAVITY	JACOB	38
C		JACOB	39
C	DATA KB, E0, H, C, PI / 8.614E-05, 1.602E-19, 6.625E-34,	JACOB	40
C	1 3.000E+10, 3.14159 /	JACOB	41
C		JACOB	42
C	IBeam = JBEAM*DEPOSIT*SHAPE(T)	JACOB	43
C	KT = KB*TMOL	JACOB	44
C	DO 1 I = 1,N	JACOB	45
C	DO 1 J = 1,N	JACOB	46
C	1 PHI(I,J) = 0.	JACOB	47
C	PHI(1,1) = - C*GAMMA	JACOB	48
C		JACOB	49
C		JACOB	50
C	CAVITY = MIRROR SEPARATION (CM)	JACOB	51
C	LENGTH = LENGTH OF ACTIVE MEDIUM (CM)	JACOB	52
C	OMEGA = AREA/CAVITY**2	JACOB	53
C	AREA = AREA OF OPTICS (CM2)	JACOB	54
C	GAMMA = [LOSS + LN(1/R)/2]/LENGTH	JACOB	55
C		JACOB	56
C	.....	JACOB	57
C		JACOB	58

Fig. 4.3: (Synthesized) Subroutine JACOB.

C	THE FOLLOWING REACTIONS DEFINE THE KINETICS --	JACOB	59
C		JACOB	60
C	1 $AR + E \rightleftharpoons AR* + E$	JACOB	61
C		JACOB	62
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	63
C	$KF(1) = VSIG(1, 1)$	JACOB	64
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	65
C	$KR(1) = VSIG(2, 1)$	JACOB	66
C		JACOB	67
C	$R = KF(1)*NO(3) - KR(1)*NO(4)$	JACOB	68
C		JACOB	69
C	$PHI(3, 2) = PHI(3, 2) - R$	JACOB	70
C	$PHI(4, 2) = PHI(4, 2) + R$	JACOB	71
C		JACOB	72
C	$R = KF(1)*NO(2)$	JACOB	73
C		JACOB	74
C	$PHI(3, 3) = PHI(3, 3) - R$	JACOB	75
C	$PHI(4, 3) = PHI(4, 3) + R$	JACOB	76
C		JACOB	77
C	$R = -KR(1)*NO(2)$	JACOB	78
C		JACOB	79
C	$PHI(3, 4) = PHI(3, 4) - R$	JACOB	80
C	$PHI(4, 4) = PHI(4, 4) + R$	JACOB	81
C		JACOB	82
C	2 $KR + E \rightleftharpoons KR* + E$	JACOB	83
C		JACOB	84
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	85
C	$KF(2) = VSIG(1, 2)$	JACOB	86
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	87
C	$KR(2) = VSIG(2, 2)$	JACOB	88
C		JACOB	89
C	$R = KF(2)*NO(5) - KR(2)*NO(6)$	JACOB	90
C		JACOB	91
C	$PHI(5, 2) = PHI(5, 2) - R$	JACOB	92
C	$PHI(6, 2) = PHI(6, 2) + R$	JACOB	93
C		JACOB	94
C	$R = KF(2)*NO(2)$	JACOB	95
C		JACOB	96
C	$PHI(5, 5) = PHI(5, 5) - R$	JACOB	97
C	$PHI(6, 5) = PHI(6, 5) + R$	JACOB	98
C		JACOB	99
C	$R = -KR(2)*NO(2)$	JACOB	100
C		JACOB	101
C	$PHI(5, 6) = PHI(5, 6) - R$	JACOB	102
C	$PHI(6, 6) = PHI(6, 6) + R$	JACOB	103
C		JACOB	104
C	3 $AR + E \rightleftharpoons AR** + E$	JACOB	105
C		JACOB	106
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	107
C	$KF(3) = VSIG(1, 3)$	JACOB	108
C	REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	109
C	$KR(3) = VSIG(2, 3)$	JACOB	110
C		JACOB	111
C	$R = KF(3)*NO(3) - KR(3)*NO(7)$	JACOB	112
C		JACOB	113
C	$PHI(3, 2) = PHI(3, 2) - R$	JACOB	114
C	$PHI(7, 2) = PHI(7, 2) + R$	JACOB	115

Fig. 4.3: (Continued)

C		JACOB	192
C	7	JACOB	193
C		JACOB	194
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	195
	KF( 7) = VSIG(1, 7)	JACOB	196
C		JACOB	197
	R = KF(7)*NO(3)	JACOB	198
C		JACOB	199
	PHI( 2, 2) = PHI( 2, 2) + R	JACOB	200
	PHI( 3, 2) = PHI( 3, 2) - R	JACOB	201
	PHI( 9, 2) = PHI( 9, 2) + R	JACOB	202
C		JACOB	203
	R = KF(7)*NO(2)	JACOB	204
C		JACOB	205
	PHI( 2, 3) = PHI( 2, 3) + R	JACOB	206
	PHI( 3, 3) = PHI( 3, 3) - R	JACOB	207
	PHI( 9, 3) = PHI( 9, 3) + R	JACOB	208
C		JACOB	209
C		JACOB	294
C	13	JACOB	295
C		JACOB	296
C	FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS	JACOB	297
	KF( 13) = VSIG(1,13)	JACOB	298
C		JACOB	299
	R = KF(13)*NO(11)	JACOB	300
C		JACOB	301
	PHI( 2, 2) = PHI( 2, 2) - R	JACOB	302
	PHI( 3, 2) = PHI( 3, 2) + R	JACOB	303
	PHI( 4, 2) = PHI( 4, 2) + R	JACOB	304
	PHI(11, 2) = PHI(11, 2) - R	JACOB	305
C		JACOB	306
	R = KF(13)*NO(2)	JACOB	307
C		JACOB	308
	PHI( 2,11) = PHI( 2,11) - R	JACOB	309
	PHI( 3,11) = PHI( 3,11) + R	JACOB	310
	PHI( 4,11) = PHI( 4,11) + R	JACOB	311
	PHI(11,11) = PHI(11,11) - R	JACOB	312
C		JACOB	313
C		JACOB	351
C	16	JACOB	352
C		JACOB	353
	R = KF(16)*NO(16)	JACOB	354
C		JACOB	355
	PHI( 3, 2) = PHI( 3, 2) + R + R	JACOB	356
	PHI(16, 2) = PHI(16, 2) - R	JACOB	357
C		JACOB	358
	R = KF(16)*NO(2)	JACOB	359
C		JACOB	360
	PHI( 3,16) = PHI( 3,16) + R + R	JACOB	361
	PHI(16,16) = PHI(16,16) - R	JACOB	362
C		JACOB	363

Fig. 4.3: (Continued)



C		JACOB	383
C	19 AR + ME- + AR* + ME-	JACOB	384
C		JACOB	385
	R = KF(19)*IBEAM/E0	JACOB	386
C		JACOB	387
	PHI( 3, 3) = PHI( 3, 3) - R	JACOB	388
	PHI( 4, 3) = PHI( 4, 3) + R	JACOB	389
C		JACOB	390
	R = -KR(19)*IBEAM/E0	JACOB	391
C		JACOB	392
	PHI( 3, 4) = PHI( 3, 4) - R	JACOB	393
	PHI( 4, 4) = PHI( 4, 4) + R	JACOB	394
C		JACOB	395
C	20 KR + ME- + KR(+) + ME- + E	JACOB	396
C		JACOB	397
	R = KF(20)*IBEAM/E0	JACOB	398
C		JACOB	399
	PHI( 2, 5) = PHI( 2, 5) + R	JACOB	400
	PHI( 5, 5) = PHI( 5, 5) - R	JACOB	401
	PHI(10, 5) = PHI(10, 5) + R	JACOB	402
C		JACOB	403
C		JACOB	443
C	24 KR(+) + KR + M + KR2(+) + M	JACOB	444
C		JACOB	445
	R = KF(24)*NO(10)*NTOT	JACOB	446
C		JACOB	447
	PHI( 5, 5) = PHI( 5, 5) - R	JACOB	448
	PHI(10, 5) = PHI(10, 5) - R	JACOB	449
	PHI(12, 5) = PHI(12, 5) + R	JACOB	450
C		JACOB	451
	R = KF(24)*NO(5)*NTOT	JACOB	452
C		JACOB	453
	PHI( 5,10) = PHI( 5,10) - R	JACOB	454
	PHI(10,10) = PHI(10,10) - R	JACOB	455
	PHI(12,10) = PHI(12,10) + R	JACOB	456
C		JACOB	457
C		JACOB	471
C	26 AR(+) + KR + AR + KR(+) +	JACOB	472
C		JACOB	473
	REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --	JACOB	474
C		JACOB	475
	E1 = + E( 9) + E( 5)	JACOB	476
	E2 = + E( 3) + E(10)	JACOB	477
	KR( 26) = KF( 26)*EXP(-(E1-E2)/KT)	JACOB	478
C		JACOB	479
	R = -KR(26)*NO(10)	JACOB	480
C		JACOB	481
	PHI( 3, 3) = PHI( 3, 3) + R	JACOB	482
	PHI( 5, 3) = PHI( 5, 3) - R	JACOB	483
	PHI( 9, 3) = PHI( 9, 3) - R	JACOB	484
	PHI(10, 3) = PHI(10, 3) + R	JACOB	485
C		JACOB	486
	R = KF(26)*NO(9)	JACOB	487
C		JACOB	488
	PHI( 3, 5) = PHI( 3, 5) + R	JACOB	489
	PHI( 5, 5) = PHI( 5, 5) - R	JACOB	490
	PHI( 9, 5) = PHI( 9, 5) - R	JACOB	491
	PHI(10, 5) = PHI(10, 5) + R	JACOB	492
C		JACOB	493

Fig. 4.3 (Continued)

C	R = KF(26)*NO(5)	JACOB	494
C	PHI( 3, 9) = PHI( 3, 9) + R	JACOB	495
	PHI( 5, 9) = PHI( 5, 9) - R	JACOB	496
	PHI( 9, 9) = PHI( 9, 9) - R	JACOB	497
	PHI(10, 9) = PHI(10, 9) + R	JACOB	498
C		JACOB	499
	R = -KR(26)*NO(3)	JACOB	500
C		JACOB	501
	PHI( 3,10) = PHI( 3,10) + R	JACOB	502
	PHI( 5,10) = PHI( 5,10) - R	JACOB	503
	PHI( 9,10) = PHI( 9,10) - R	JACOB	504
	PHI(10,10) = PHI(10,10) + R	JACOB	505
C		JACOB	506
		JACOB	507
C		JACOB	1009
C 50	AR2* + AR2* + AR2(+) + AR + AR + E	JACOB	1010
C		JACOB	1011
	R = 2.*KF(50)*NO(16)	JACOB	1012
C		JACOB	1013
	PHI( 2,16) = PHI( 2,16) + R	JACOB	1014
	PHI( 3,16) = PHI( 3,16) + R + R	JACOB	1015
	PHI(11,16) = PHI(11,16) + R	JACOB	1016
	PHI(16,16) = PHI(16,16) - R - R	JACOB	1017
C		JACOB	1018
C 66	KR* + M + KR* + M	JACOB	1395
C		JACOB	1396
C	REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --	JACOB	1397
C		JACOB	1398
	E1 = + E( 8)	JACOB	1399
	E2 = + E( 6)	JACOB	1400
	KR( 66) = KF( 66)*EXP(-(E1-E2)/KT)	JACOB	1401
C		JACOB	1402
	R = -KR(66)*NTOT	JACOB	1403
C		JACOB	1404
	PHI( 6, 6) = PHI( 6, 6) + R	JACOB	1405
	PHI( 8, 6) = PHI( 8, 6) - R	JACOB	1406
C		JACOB	1407
	R = KF(66)*NTOT	JACOB	1408
C		JACOB	1409
	PHI( 6, 8) = PHI( 6, 8) + R	JACOB	1410
	PHI( 8, 8) = PHI( 8, 8) - R	JACOB	1411
C		JACOB	1412
C 67	ANF* + AR + F	JACOB	1413
C		JACOB	1414
	R = KF(67)	JACOB	1415
C		JACOB	1416
	PHI( 3,20) = PHI( 3,20) + R	JACOB	1417
	PHI(14,20) = PHI(14,20) + R	JACOB	1418
	PHI(20,20) = PHI(20,20) - R	JACOB	1419
C		JACOB	1420
C		JACOB	1467
C 74	KRF* + KR + F + HNU	JACOB	1468
C		JACOB	1469
	R = KF(74)	JACOB	1470
C		JACOB	1471
	PHI( 5,22) = PHI( 5,22) + R	JACOB	1472
	PHI(14,22) = PHI(14,22) + R	JACOB	1473
	PHI(22,22) = PHI(22,22) - R	JACOB	1474
C		JACOB	1475
C	PHOTON NUMBER DENSITY INCREASED BY NOISE --	JACOB	1476
C		JACOB	1477
	R = R*OMEGA/4./PI	JACOB	1478
	PHI(1,22) = PHI(1,22) + R	JACOB	1479

Fig. 4.3 (Continued)

C			JACOB	1480
C	75	KRF* + RAD + KR + F + RAD	JACOB	1481
C			JACOB	1482
C		(STIMULATED EMISSION PROCESS, WITH NO( 1) = INTEN/C/HNU)	JACOB	1483
C			JACOB	1484
		R = KF(75)*NO(22)	JACOB	1485
		R = R*C	JACOB	1486
C			JACOB	1487
		PHI( 1, 1) = PHI( 1, 1) + R	JACOB	1488
		PHI( 5, 1) = PHI( 5, 1) + R	JACOB	1489
		PHI(14, 1) = PHI(14, 1) + R	JACOB	1490
		PHI(22, 1) = PHI(22, 1) - R	JACOB	1491
C			JACOB	1492
		R = KF(75)*NO(1)	JACOB	1493
		R = R*C	JACOB	1494
C			JACOB	1495
		PHI( 1,22) = PHI( 1,22) + R	JACOB	1496
		PHI( 5,22) = PHI( 5,22) + R	JACOB	1497
		PHI(14,22) = PHI(14,22) + R	JACOB	1498
		PHI(22,22) = PHI(22,22) - R	JACOB	1499
C			JACOB	1500
C	76	F2 + RAD + F + F	JACOB	1501
C			JACOB	1502
C		(RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)	JACOB	1503
C			JACOB	1504
		R = KF(76)*NO(13)	JACOB	1505
		R = R*C	JACOB	1506
C			JACOB	1507
		PHI( 1, 1) = PHI( 1, 1) - R	JACOB	1508
		PHI(13, 1) = PHI(13, 1) - R	JACOB	1509
		PHI(14, 1) = PHI(14, 1) + R + R	JACOB	1510
C			JACOB	1511
		R = KF(76)*NO(1)	JACOB	1512
		R = R*C	JACOB	1513
C			JACOB	1514
		PHI( 1,13) = PHI( 1,13) - R	JACOB	1515
		PHI(13,13) = PHI(13,13) - R	JACOB	1516
		PHI(14,13) = PHI(14,13) + R + R	JACOB	1517
C			JACOB	1518
C	77	F- + RAD + F + E	JACOB	1519
C			JACOB	1520
C		(RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)	JACOB	1521
C			JACOB	1522
		R = KF(77)*NO(15)	JACOB	1523
		R = R*C	JACOB	1524
C			JACOB	1525
		PHI( 1, 1) = PHI( 1, 1) - R	JACOB	1526
		PHI( 2, 1) = PHI( 2, 1) + R	JACOB	1527
		PHI(14, 1) = PHI(14, 1) + R	JACOB	1528
		PHI(15, 1) = PHI(15, 1) - R	JACOB	1529
C			JACOB	1530
		R = KF(77)*NO(1)	JACOB	1531
		R = R*C	JACOB	1532
C			JACOB	1533
		PHI( 1,15) = PHI( 1,15) - R	JACOB	1534
		PHI( 2,15) = PHI( 2,15) + R	JACOB	1535
		PHI(14,15) = PHI(14,15) + R	JACOB	1536
		PHI(15,15) = PHI(15,15) - R	JACOB	1537
C			JACOB	1538
C	78	KH2F* + RAD + AR* + KR + F	JACOB	1539
C			JACOB	1540

Fig. 4.3 (Continued)



C	(RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)	JACOB	1541
C	R = KF(78)*NO(23)	JACOB	1542
	R = R*C	JACOB	1543
C	PHI( 1, 1) = PHI( 1, 1) - R	JACOB	1544
	PHI( 4, 1) = PHI( 4, 1) + R	JACOB	1545
	PHI( 5, 1) = PHI( 5, 1) + R	JACOB	1546
	PHI(14, 1) = PHI(14, 1) + R	JACOB	1547
	PHI(23, 1) = PHI(23, 1) - R	JACOB	1548
C	R = KF(78)*NO(1)	JACOB	1549
	R = R*C	JACOB	1550
C	PHI( 1,23) = PHI( 1,23) - R	JACOB	1551
	PHI( 4,23) = PHI( 4,23) + R	JACOB	1552
	PHI( 5,23) = PHI( 5,23) + R	JACOB	1553
	PHI(14,23) = PHI(14,23) + R	JACOB	1554
	PHI(23,23) = PHI(23,23) - R	JACOB	1555
C	79 AR2(*) + RAD = AR + AR(*)	JACOB	1556
C	(RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)	JACOB	1557
C	R = KF(79)*NO(11)	JACOB	1558
	R = R*C	JACOB	1559
C	PHI( 1, 1) = PHI( 1, 1) - R	JACOB	1560
	PHI( 3, 1) = PHI( 3, 1) + R	JACOB	1561
	PHI( 9, 1) = PHI( 9, 1) + R	JACOB	1562
	PHI(11, 1) = PHI(11, 1) - R	JACOB	1563
C	R = KF(79)*NO(1)	JACOB	1564
	R = R*C	JACOB	1565
C	PHI( 1,11) = PHI( 1,11) - R	JACOB	1566
	PHI( 3,11) = PHI( 3,11) + R	JACOB	1567
	PHI( 9,11) = PHI( 9,11) + R	JACOB	1568
	PHI(11,11) = PHI(11,11) - R	JACOB	1569
C	80 KR2(*) + RAD = KR + KR(*)	JACOB	1570
C	(RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)	JACOB	1571
C	R = KF(80)*NO(12)	JACOB	1572
	R = R*C	JACOB	1573
C	PHI( 1, 1) = PHI( 1, 1) - R	JACOB	1574
	PHI( 5, 1) = PHI( 5, 1) + R	JACOB	1575
	PHI(10, 1) = PHI(10, 1) + R	JACOB	1576
	PHI(12, 1) = PHI(12, 1) - R	JACOB	1577
C	R = KF(80)*NO(1)	JACOB	1578
	R = R*C	JACOB	1579
C	PHI( 1,12) = PHI( 1,12) - R	JACOB	1580
	PHI( 5,12) = PHI( 5,12) + R	JACOB	1581
		JACOB	1582
		JACOB	1583
		JACOB	1584
		JACOB	1585
		JACOB	1586
		JACOB	1587
		JACOB	1588
		JACOB	1589
		JACOB	1590
		JACOB	1591
		JACOB	1592
		JACOB	1593
		JACOB	1594
		JACOB	1595
		JACOB	1596
		JACOB	1597

Fig. 4.3 (Continued)

	PHI(10,12) = PHI(10,12) + R	JACOB	1598
	PHI(12,12) = PHI(12,12) - R	JACOB	1599
C		JACOB	1600
	RATIO = LENGTH/CAVITY	JACOB	1601
	DO 3 I = 1,N	JACOB	1602
	3 PHI(1,I) = RATIO*PHI(1,I)	JACOB	1603
C		JACOB	1604
C	.....	JACOB	1605
C		JACOB	1606
C	EXTERNAL CIRCUIT EQUATIONS (Q = NO(25), AND I = NO(26)) --	JACOB	1607
C		JACOB	1608
	NE = NO(2)	JACOB	1609
	IF (NE.EQ.0.) NE = 1.0	JACOB	1610
	CONDUCT = NE*E0*MU	JACOB	1611
	RD = D/AREA/CONDUCT	JACOB	1612
C		JACOB	1613
	IF (L0.EQ.0.) GO TO 2	JACOB	1614
	PHI(25,25) = 0.	JACOB	1615
	PHI(25,26) = 1.0	JACOB	1616
	PHI(26,25) = -1./L0/C0	JACOB	1617
	PHI(26,26) = -(R0 + RD)/L0	JACOB	1618
	PHI(26, 2) = NO(26)*RD/NE/L0	JACOB	1619
	RETURN	JACOB	1620
C		JACOB	1621
	2 PHI(25,25) = DIDQ = - 1./C0/(R0 + RD)	JACOB	1622
	PHI(25, 2) = NO(25)*DIDQ*RD/NE/(R0 + RD)	JACOB	1623
C		JACOB	1624
C	.....	JACOB	1625
C		JACOB	1626
C	THE FOLLOWING MOLECULAR SPECIES (WITH LABELS) WERE INCLUDED --	JACOB	1627
C		JACOB	1628
C	1 RAD                    2 E(-)                    3 AR                    4 AR*	JACOB	1629
C	5 KR                    6 KR*                    7 AR**                    8 KR**	JACOB	1630
C	9 AR(+)                    10 KR(+)                    11 AR2(+)                    12 KR2(+)                    13 F2                    14 F                    15 F-                    16 AR2*	JACOB	1631
C	17 KR2*                    18 ARKR(+)                    19 ARKR*                    20 ARF*	JACOB	1632
C	21 AR2F*                    22 KRF*                    23 KR2F*                    24 ARKRF*	JACOB	1633
C		JACOB	1634
C		JACOB	1635
C	.....	JACOB	1636
C		JACOB	1637
	RETURN	JACOB	1638
	END	JACOB	1639

Fig. 4.3 (Continued)

	SUBROUTINE LEVELS (N1, N2, NO)	LEVELS	2
C	.....	LEVELS	3
C		LEVELS	4
C	THIS SUBROUTINE DETERMINES THE POPULATION DENSITIES N1(I), N2(I)	LEVELS	5
C	OF THE (LOWER AND UPPER) LEVELS INVOLVED IN THE ITH INELASTIC	LEVELS	6
C	SCATTERING PROCESS INCLUDED IN THE COUPLED E- KINETICS ANALYSIS.	LEVELS	7
C		LEVELS	8
C	THE GENERAL KINETICS SYNTHESIS PROGRAM WHICH AUTOMATICALLY GEN-	LEVELS	9
C	ERATED THIS SUBROUTINE WAS DEVELOPED BY --	LEVELS	10
C		LEVELS	11
C		LEVELS	12
C	-----	LEVELS	13
C	I	LEVELS	14
C	I DR. WILLIAM B. LACINA	LEVELS	15
C	I NORTHROP RESEARCH AND TECHNOLOGY	LEVELS	16
C	I ONE RESEARCH PARK	LEVELS	17
C	I PALOS VERDES PENINSULA, CA 90274	LEVELS	18
C	I TEL: (213) 377-4811, EXT. 322	LEVELS	19
C	I	LEVELS	20
C	-----	LEVELS	21
C	.....	LEVELS	22
C		LEVELS	23
C	REAL N1(1), N2(1), NO(1)	LEVELS	24
C		LEVELS	25
C	N1( 1) = NO( 3)	LEVELS	26
C	N2( 1) = NO( 4)	LEVELS	27
C		LEVELS	28
C	N1( 2) = NO( 5)	LEVELS	29
C	N2( 2) = NO( 6)	LEVELS	30
C		LEVELS	31
C	N1( 3) = NO( 3)	LEVELS	32
C	N2( 3) = NO( 7)	LEVELS	33
C		LEVELS	34
C	N1( 4) = NO( 5)	LEVELS	35
C	N2( 4) = NO( 8)	LEVELS	36
C		LEVELS	37
C	N1( 5) = NO( 4)	LEVELS	38
C	N2( 5) = NO( 7)	LEVELS	39
C		LEVELS	40
C	N1( 6) = NO( 6)	LEVELS	41
C	N2( 6) = NO( 8)	LEVELS	42
C		LEVELS	43
C	N1( 7) = NO( 3)	LEVELS	44
C	N2( 7) = 0.	LEVELS	45
C		LEVELS	46
C	N1( 8) = NO( 5)	LEVELS	47
C	N2( 8) = 0.	LEVELS	48
C		LEVELS	49
C	N1( 9) = NO( 4)	LEVELS	50
C	N2( 9) = 0.	LEVELS	51
C		LEVELS	52
C	N1(10) = NO( 6)	LEVELS	53
C	N2(10) = 0.	LEVELS	54
C		LEVELS	55
C	N1(11) = NO( 7)	LEVELS	56
C	N2(11) = 0.	LEVELS	57
C		LEVELS	58
C	N1(12) = NO( 8)	LEVELS	59
C	N2(12) = 0.	LEVELS	60
C		LEVELS	61
C	N1(13) = NO(11)	LEVELS	62
C	N2(13) = 0.	LEVELS	63
C		LEVELS	64
C	N1(14) = NO(12)	LEVELS	65
C	N2(14) = 0.	LEVELS	66
C		LEVELS	67
C	N1(15) = NO(13)	LEVELS	68
C	N2(15) = 0.	LEVELS	69
C		LEVELS	70
C	RETURN	LEVELS	71
C	END	LEVELS	72
		LEVELS	73

Fig. 4.4 (Synthesized) Subroutine LEVELS



# SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CH3/SEC, CM6/SEC, .... OR CH2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

1	REACTION(1) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(1)	KR(1)	RATE REFERENCES AND/OR COMMENTS
1	AR + E → AR* + F	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, REITRAGE AUS PLASMA PHYS 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
2	KR + E → KR* + F	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, REITRAGE AUS PLASMA PHYS 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
3	AR + E → AR** + F	(COMPUTED)	(COMPUTED)	0.1 X CROSS SECTION FOR AR + E → AR* + E IS ASSUME FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
4	KR + E → KR** + E	(COMPUTED)	(COMPUTED)	0.1 X CROSS SECTION FOR KR + E → KR* + E IS ASSUME FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
5	AR* + E → AR** + E	(COMPUTED)	(COMPUTED)	VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
6	KR* + E → KR** + E	(COMPUTED)	(COMPUTED)	VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
7	AR + E → AR(*) + E + E	(COMPUTED)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
8	KR + E → KR(*) + E + E	(COMPUTED)		KIEFFER REPORT, P. 16 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
9	AR* + E → AR(*) + E + E	(COMPUTED)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
10	KR* + E → KR(*) + E + E	(COMPUTED)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY, DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme.

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1), CM3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

1 REACTION(1)  
(IGNORED REACTIONS ARE NOT NUMBERED)

RATE CONSTANTS  
KF(1) KR(1)

RATE REFERENCES AND/OR COMMENTS

11	AR** + E → AR(1) + E + E	(COMPUTED)	VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR ≠ 0.
12	KR** + E → KR(1) + E + E	(COMPUTED)	VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR ≠ 0.
13	AR2(1) + E → AR* + AR	(COMPUTED)	MEHR AND BIONDI: SYNTHETIC CROSS SECTION FOR TE** FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR ≠ 0.
14	KR2(1) + E → KR* + KR	(COMPUTED)	OSKAM, MITTELSTADT: SYNTHETIC, TE**(-2/3) LAW. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR ≠ 0.
15	F2 + E → F + F-	(COMPUTED)	AEROSPACE (PRIVATE COMM.) FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR ≠ 0.
16	AR2* + E → AR + AR + E	1.0000E-07	REVERSE REACTION IS IGNORED -- KR ≠ 0.
17	KR2* + E → KR + KR + E	1.0000E-07	REVERSE REACTION IS IGNORED -- KR ≠ 0.
18	AR + HE- → AR(1) + HE- + E	4.3400E-18	BERGER-SELTZER STOP @ 1.7 MEVCM2/GM (300 KEV) E- CREATION ASSUMED TO BE OVER ENERGY DISTRIBUTION REVERSE REACTION IS IGNORED -- KR ≠ 0.
19	AR + HE- → AR* + HE-	1.2400E-18	(1/3.5) × AR + HE → AR(1) + E + HE
20	KR + HE- → KR(1) + HE- + E	8.0400E-18	BERGER-SELTZER STOP @ 1.5 MEVCM2/GM (300 KEV) E- CREATION ASSUMED TO BE OVER ENERGY DISTRIBUTION REVERSE REACTION IS IGNORED -- KR ≠ 0.
21	KR + HE- → KR* + HE-	2.3000E-18	(1/3.5) × KR + HE → KR(1) + E + HE
22	AR(1) + AR + M → AR2(1) + M	2.0000E-31	W. F. LIU, D. C. CONWAY JCP 62, 3070 (1975) REVERSE REACTION IS IGNORED -- KR ≠ 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1), CM3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS		RATE REFERENCES AND/OR COMMENTS
		KF(I)	KR(I)	
23	AR(*) + KR + M → ARKR(*) + M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
24	KR(*) + KR + M → KR2(*) + M	2.4000E-31		C. J. TRACY, M. J. OSKAM JCP 65, 3387 (1976) REVERSE REACTION IS IGNORED -- KR = 0.
25	KR(*) + AR + M → ARKR(*) + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
26	AR(*) + KR + AR → KR(*)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
27	AR2(*) + KR → KR(*) + AR + AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970) REVERSE REACTION IS IGNORED -- KR = 0.
28	ARKR(*) + KR → KR2(*) + AR	3.2000E-10	X E(-E/KT)	BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
29	AR* + AR + M → AR2* + M	1.0000E-32		HILL, GUTCHECK, MUESTIS, ET AL, SRI REPORT, 1974. REVERSE REACTION IS IGNORED -- KR = 0.
30	AR* + KR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
31	KR* + KR + M → KR2* + M	5.5000E-32		HUGHES LASL ASPEN 9/76 REVERSE REACTION IS IGNORED -- KR = 0.
32	KR* + AR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
33	ARKR* + KR → KR2* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
34	AR2(*) + F- → ARF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
35	AR2(*) + F- → AR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
36	AR(*) + F- → ARF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
37	KR2(*) + F- → KRF* + KR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
38	KR2(*) + F- → KR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
39	KR(*) + F- → KRF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
40	ARKR(*) + F- → KRF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).



SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, .... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS		RATE REFERENCES AND/OR COMMENTS
		KF(I)	KR(I)	
41	ARKR(+) * F - * ARKRF*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
42	KR* * F2 * KRF* * F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
43	AR* * F2 * ARF* * F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
44	AR* * KR * AR * KR*	6.2000E-12	X E(-E/KT)	PIPER, SETSER, CLYNE, JCP 63, 4018 (1975) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
45	KRF* * AR * M * ARKRF* * M	6.0000E-32		AVCO REVERSE REACTION IS IGNORED -- KR = 0.
46	KRF* * KR * M * KR2F* * M	5.0000E-31		AVCO REVERSE REACTION IS IGNORED -- KR = 0.
47	ARF* * AR * M * AR2F* * M	4.0000E-31		AVCO REVERSE REACTION IS IGNORED -- KR = 0.
48	ARF* * KR * M * ARKRF* * M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
49	AR2* * KR * AR * AR * KR*	8.0000E-11		ZAMIR (PRIV. COMMUN. TO SRI) REVERSE REACTION IS IGNORED -- KR = 0.
50	AR2* * AR2* * AR2(+) * AR * AR * E	3.0000E-10		E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
51	ARF* * KR * KRF* * AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
52	AR2* * F * ARF* * AR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
53	KR2* * F * KRF* * KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
54	AR2* * F2 * AR2F* * F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
55	ARKR* * F2 * KRF* * AR * F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTIONS(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS		RATE REFERENCES AND/OR COMMENTS
		KF(I)	KR(I)	
56	ARKR* + F2 + ARKR* + F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
57	KR2* + F2 + KR2F* + F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
58	AR2F* + F2 + AR + AR* + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
59	ARKRF* + F2 + AR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
60	KR2F* + F2 + KR + KR* + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
61	ARKRF* + KR + KR2F* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
62	KRF* + F2 + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
63	ARF* + F2 + AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
64	AR2F* + KR + KRF* + AR + AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
65	AR* + M + AR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
66	KR* + M + KR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
67	ARF* + AR + F	3.3000E+07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
68	AR2* + AR + AR	3.8000E+06		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
69	ARKR* + AR + KR	3.0000E+06		REVERSE REACTION IS IGNORED -- KR = 0.
70	KR2* + KR + KR	3.3000E+06		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
71	AR2F* + AR + AR + F	2.0000E+08		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, .... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
(IGNORED REACTIONS ARE NOT NUMBERED)				
72	ARKF* + AR + KR + F	5.0000E-07		SRI REPORT NO. HP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
73	KR2F* + KR + KR + F	6.7000E-07		SRI REPORT NO. HP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
74	KRF* + KR + F + HNU	1.1000E-08		R. BURNHAM, S. S. SEARLES (SUBMITTED TO JCP) REVERSE REACTION IS IGNORED -- KR = 0. NO REVERSE REACTION ALLOWED FOR RADIATIVE DECAY.
75	KRF* + RAD + KR + F + RAD	2.0000E-16		LASER TRANSITION'S STIMULATED EMISSION X-SECTION REVERSE REACTION IS IGNORED -- KR = 0.
76	F2 + RAD + F + F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
77	F- + RAD + F + E	5.4000E-18		A. MANDL, PHYS REV A3, 251 (1971) E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
78	KR2F* + RAD + AR* + KR + F	1.0000E-99		CROSS SECTION UNKNOWN REVERSE REACTION IS IGNORED -- KR = 0.
79	AR2(+) + RAD + AR + AR(+)	1.5000E-17		STEVENS (PARK CITY CONFERENCE) REVERSE REACTION IS IGNORED -- KR = 0.
80	KR2(+) + RAD + KR + KR(+)	3.5000E-18		J. WEST (NRTC) REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

OF 80 INPUT REACTIONS SCANNED, 80 WERE RETAINED (MAXIMUM ALLOWED = 200) AND 0 WERE IGNORED FOR REASONS ITEMIZED IN THE TABLE.  
OF THOSE RETAINED, 15 REQUIRE RATES FROM AN E- KINETICS ANALYSIS. 24 SEPARATE SPECIES WERE ENCOUNTERED (MAXIMUM ALLOWED = 30).

Fig. 4.5: Summary of input reaction scheme (cont'd).



SUMMARY OF REACTIONS FOR WHICH EACH SPECIES OCCURS: NTYPE = 24  
(THIS EDIT PERMITS RAPID DELETION OF ANY SPECIES FROM THE KINETIC SYSTEM)

I	GAS(I)	REACTIONS CONTAINING GAS(I)																			
		75,	76,	77,	78,	79,	80,														
1	RAO	75,	76,	77,	78,	79,	80,														
2	E(-)	1,	2,	3,	4,	5,	6,	7,	8,	9,	10,	11,	12,	13,	14,	15,	16,	17,	18,	20,	50
3	AR	1,	3,	7,	13,	16,	18,	19,	22,	25,	26,	27,	28,	29,	32,	33,	34,	40,	44,	45,	47
4	AR*	49,	50,	51,	52,	55,	58,	59,	61,	63,	64,	67,	68,	69,	71,	72,	79,				
5	KR	1,	5,	9,	13,	19,	29,	30,	43,	44,	65,	78,									
6	KR*	2,	4,	8,	14,	17,	20,	21,	23,	24,	26,	27,	28,	30,	31,	33,	37,	44,	46,	48,	49
7	AR**	51,	53,	59,	60,	61,	62,	64,	69,	70,	72,	73,	74,	75,	78,	80,					
8	KR**	2,	6,	10,	14,	21,	31,	32,	42,	44,	49,	66,									
9	AR(+)	3,	5,	11,	65,																
10	KR(+)	4,	6,	12,	66,																
11	AR2(+)	7,	9,	11,	18,	22,	23,	26,	36,	79,											
12	KR2(+)	8,	10,	12,	20,	24,	25,	26,	27,	39,	80,										
13	F2	13,	22,	27,	34,	35,	50,	79,													
14	F	14,	24,	28,	37,	38,	80,														
15	F-	15,	42,	43,	54,	55,	56,	57,	58,	59,	60,	62,	63,	76,							
16	AR2*	15,	42,	43,	52,	53,	54,	55,	56,	57,	58,	59,	60,	62,	63,	76,					
17	KR2*	76,	77,	78,																	
18	ARKR(+)	15,	34,	35,	36,	37,	38,	39,	40,	41,	77,										
19	ARKR*	16,	29,	49,	50,	52,	54,	68,													
		17,	31,	33,	53,	57,	70,														
		23,	25,	28,	40,	41,															
		30,	32,	33,	55,	56,	69,														

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.6: Cross-reference table between species and reactions.

SUMMARY OF REACTIONS FOR WHICH EACH SPECIES OCCURS: NTYPE = 24  
(THIS EDIT PERMITS RAPID DELETION OF ANY SPECIES FROM THE KINETIC SYSTEM)

REACTIONS CONTAINING GAS(1)

1 GAS(1)

20	ARF*	34, 36, 43, 47, 48, 51, 52, 63, 67,
21	AR2F*	35, 47, 54, 58, 64, 71,
22	KRF*	37, 39, 40, 42, 45, 46, 51, 53, 55, 62, 64, 74, 75,
23	KR2F*	38, 46, 57, 60, 61, 73, 78,
24	ARKRF*	41, 45, 48, 56, 59, 61, 72,

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.6: Cross-reference table between species and reactions (cont'd).

(as indicated in Fig.3.5) or directly (with the control card deck given in Fig. 3.6). Fig. 4.7 shows the "playback" (generated in output by subroutine EDITOR) of the exact input card images of DATA BLOCK 4, which specifies the experimental conditions. The structure of the input deck has been described in Sec. 3.2 and summarized in Tables 3.4 - 3.10.

At the beginning of the output after execution of the analysis, a cover page as shown in Fig. 4.8 (actually, two identical such pages) is generated, containing a block-letter title defined by the header card of DATA BLOCK 1 at the time of program synthesis (cf. Fig. 4.1). As described in Table 3.5, the IO input vector provided by \$CONTROL\$ entry (cf. Fig. 4.7) is used to specify output option requests. If IO(10) is nonzero, an initial summary of the reaction scheme and its rate constants (as modified by \$RATES\$ input entry) is generated, shown in Fig. 4.9. (The effect of rate modifications will be illustrated in Sec. 4.3 below.) Only the first (50 BCD character) line of comments which appeared in Fig. 4.5 is retained. If IO(8) and IO(9) had been entered nonzero, a tabular summary and plot of all inelastic and momentum transfer electron cross section data (used in the analysis) is provided, as shown in Fig. 4.10 and 4.11. The parameters IO(I), I = 1, 2, ..., 7 are used to specify the frequency of certain output options described in Table 3.5. Fig. 4.12 - 4.18 are samples of such output corresponding to cycle k = 20 ( $t = 200 \times 10^{-9}$  s). The first five of these figures summarize results of the electron kinetics analysis at  $t = 200$  ns, while the sixth (Fig. 4.17) summarizes the molecular kinetic, electrical, and optical parameters.

Note that Fig. 4.17 contains a tabulation of the population densities and their instantaneous rates of change for all of the species. Also shown



is an effective (instantaneous) time constant  $\tau_I$  for each species I,

$$\tau_I(t)^{-1} = \left| dN_I(t)/dt \right| / N_I(t),$$

which is useful for indication of how rapidly any given species is evolving at any given time. Fig. 4.18 is a (partial) reproduction of output which summarizes the numerical contribution of each kinetic reaction to every species, and is useful for assessing reaction sensitivities. If a particular reaction makes only a negligible contribution under typical conditions of interest, it can easily be deleted in a future version of the program. Since the output format of Fig. 4.12 - 4.18 is essentially self-explanatory, no further description should be necessary.

At the conclusion of the analysis, numerous parameters are plotted or tabulated as a function of time, such as  $e^-$ -beam current density (Fig. 4.19), intracavity radiation intensity (Fig. 4.20), circuit voltages and power densities (Fig. 4.21), instantaneous net gain coefficient (Fig. 4.22) and medium gain and absorption coefficients (Fig. 4.23), optical and electrical power densities (Fig. 4.24) and energy densities (Fig. 4.25), circuit voltages (Fig. 4.26), plasma conductivity and discharge impedance (Fig. 4.27), discharge current density (Fig. 4.28), optically extracted power (Fig. 4.29) and energy (Fig. 4.30) density and efficiency, and the population densities (and rates of change) for miscellaneous species as requested (Fig. 4.31 - 4.35).

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK  
(DATE: 01/12/79)

CARD NO.	1	2	3	4	5	6	7	8
1	....	SCONTROL						
2	....		IO(1) = 10,20,20,20,10,10,20,0,0,1,					
3	....		EMAX = 20.,					
4	....	SPARAM	NCYCLE = 1000					
5	....		TPULSE = 1.0E-06,					
6	....	SOPTICAL	ATM = 2.05					
7	....		REFLECT = 70.,					
8	....		LOSS = 0.,					
9	....		AREA = 25.,					
10	....		CAVITY = 130.,					
11	....	SEBEAM	LENGTH = 75.05					
12	....		JBEAM = 10.0,					
13	....		ENERGY = 300.,					
14	....		UB = 20.,					
15	....		TB(1) = 0., 50., 100., 150., 200., 250., 300.,					
16	....		350., 400., 450., 500., 550., 600., 650.,					
17	....		700., 750., 800., 850., 900., 950., 1000.,					
18	....		UNITS = 1.0E-09,					
19	....		JB(1) = 0., .82, 1., 1., .9, .85, .77, .73, .69,					
20	....		.67, .69, .72, .75, .75, .72, .65, .42, .2,					
21	....		.05, .02, 0.,					
22	....	SCIRCUIT	FACTOR = 2.05,					
23	....		CAPAC = 1.00E-06,					
24	....		INDUCT = 200.E-09,					
25	....		RESIST = 0.,					
26	....		KVOLT = 50.,					
27	....		AREA = 2000.,					
28	....	SRATES \$	DIST = 10.5					
29	....	AR	89.9	40.				
30	....	KR	10.0	84.				
31	....	F2	0.1	38.				
32	....	AR*					PLOT	
33	....	KR*	11.5				PLOT	
34	....	AR2(+)	9.9				PLOT	
35	....	KR2(+)	13.0				PLOT	
36	....	ARKR(+)	11.8				PLOT	
37	....	AR*	12.8					
38	....	AR(+)	13.5					
39	....	KR*	15.8				PLOT	
40	....	KR(+)	11.5				PLOT	
			14.4					

1	2	3	4	5	6	7	8
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK  
(DATE: 01/12/79)

CARD NO.	1	2	3	4	5	6	7	8
41	....	ARF*	6.5					
42	....	KRF*	5.0					
43	....	AR2*	9.5					
44	....	KR2*	8.2					
45	....	AR2F*	5.0					
46	....	ARKRF*	4.0					
47	....	KR2F*	3.0					
48	....	ARKR*	8.8					
49	....	F-					PLOT	
50	....	E(-)					PLOT	

1	2	3	4	5	6	7	8
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

Fig. 4.7: DATA BLOCK 4 card input of numerical control values, experimental parameters, modification of rate constants, and initialization of species.

THIS CODE WAS DEVELOPED BY

DR. WILLIAM B. LACINA  
NORTHROP RESEARCH AND TECHNOLOGY  
ONE RESEARCH PARK  
PALOS VERDES PENINSULA, CA 90274  
TEL: (213) 377-4811, EXT. 322

**Fig. 4.8:** Cover page, generated at beginning of each output, with a block-letter title defined by the header card of DATA BLOCK 1 at time of program synthesis.



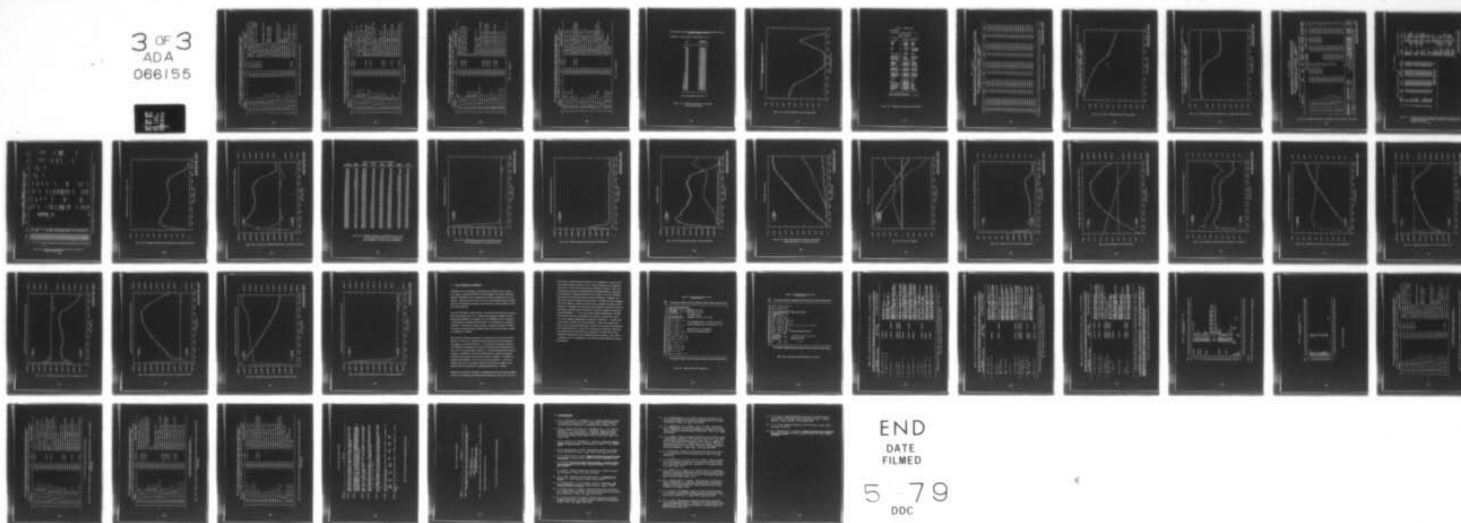
AD-A066 155

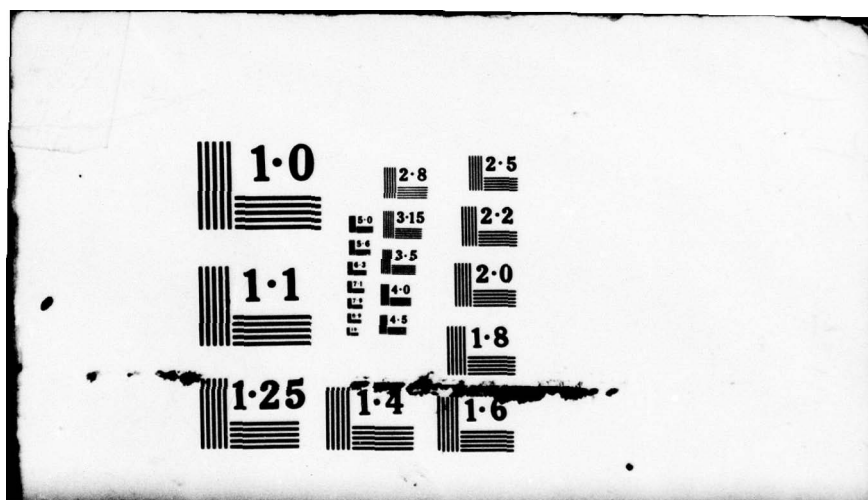
NORTHROP RESEARCH AND TECHNOLOGY CENTER PALOS VERDES --ETC F/G 20/5  
THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSES--ETC(U)  
JAN 79 W B LACINA  
N00014-78-C-0499  
NL

UNCLASSIFIED

3 OF 3  
ADA  
066155

USE





SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
 DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSI(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
1	AR + E → AR* + E	VSI(1, 1)	VSI(2, 1)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
2	KR + E → KR* + E	VSI(1, 2)	VSI(2, 2)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
3	AR + E → AR** + E	VSI(1, 3)	VSI(2, 3)	0.1 X CROSS SECTION FOR AR + E → AR* + E IS ASSUME
4	KR + E → KR** + E	VSI(1, 4)	VSI(2, 4)	0.1 X CROSS SECTION FOR KR + E → KR* + E IS ASSUME
5	AR* + E → AR** + E	VSI(1, 5)	VSI(2, 5)	VRIENS CROSS SECTION
6	KR* + E → KR** + E	VSI(1, 6)	VSI(2, 6)	VRIENS CROSS SECTION
7	AR + E → AR(•) + E + E	VSI(1, 7)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43
8	KR + E → KR(•) + E + E	VSI(1, 8)		KIEFFER REPORT, P. 16
9	AR* + E → AR(•) + E + E	VSI(1, 9)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
10	KR* + E → KR(•) + E + E	VSI(1, 10)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
11	AR** + E → AR(•) + E + E	VSI(1, 11)		VRIENS CROSS SECTION
12	KR** + E → KR(•) + E + E	VSI(1, 12)		VRIENS CROSS SECTION
13	AR2(•) + E → AR* + AR	VSI(1, 13)		MEHR AND BIONDI: SYNTHETIC CROSS SECTION FOR TE**
14	KR2(•) + E → KR* + KR	VSI(1, 14)		OSKAM, MITTELSTADT: SYNTHETIC, TE**(-2/3) LAW.
15	F2 + E → F + F-	VSI(1, 15)		AEROSPACE (PRIVATE COMMUN.)
16	AR2* + E → AR + AR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
17	KR2* + E → KR + KR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
18	AR + HE- → AR(•) + HE- + E	4.3400E-10		BERGER-SELTZER: STOP = 1.7 MEVCM2/GM (300 KEV)
19	AR + HE- → AR* + HE-	1.2400E-10	1.2400E-10	(1/3.5) X AR + HE → AR(•) + E + HE
20	KR + HE- → KR(•) + HE- + E	8.0400E-10		BERGER-SELTZER: STOP = 1.5 MEVCM2/GM (300 KEV)

Fig. 4.9: Summary of rate constants used for execution.



SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
 DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA  
 (VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
21	KR • HE- • KR • HE-	2.3000E-10	2.3000E-10	(1/3.5) X KR • HE • KR(I) • E • HE
22	AR(I) • AR • M • AR2(I) • M	2.0000E-31		W. F. LIU, D. C. CONWAY JCP 62, 3070 (1975)
23	AR(I) • KR • M • ARKR(I) • M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
24	KR(I) • KR • M • KR2(I) • M	2.4000E-31		C. J. TRACY, M. J. OSKAM JCP 65, 3387 (1976)
25	KR(I) • AR • M • ARKR(I) • M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
26	AR(I) • KR • AR • KR(I)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
27	AR2(I) • KR • KR(I) • AR • AR	7.5000E-10		BONNE ET AL, J. CHEM. PHYS. 52, 5094 (1970)
28	ARKR(I) • KR • KR2(I) • AR	3.2000E-10	X E(-E/KT)	BONNE ET AL, J. CHEM. PHYS. 52, 5094 (1970)
29	AR • AR • M • AR2 • M	1.0000E-32		HILL, GUTCHECK, MUESTIS, ET AL, SRI REPORT, 1974.
30	AR • KR • M • ARKR • M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
31	KR • KR • M • KR2 • M	5.5000E-32		HUGHES LASL ASPEN 9/76
32	KR • AR • M • ARKR • M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
33	ARKR • KR • KR2 • AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
34	AR2(I) • F- • ARF • AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
35	AR2(I) • F- • AR2F •	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
36	AR(I) • F- • ARF •	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
37	KR2(I) • F- • KRF • KR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
38	KR2(I) • F- • KR2F •	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
39	KR(I) • F- • KRF •	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
40	ARKR(I) • F- • KRF • AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

Fig. 4.9: Continued

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
41	ARKR(*) + F - ARKR*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
42	KR* + F2 + KRF* + F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
43	AR* + F2 + ARF* + F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
44	AR* + KR + AR + KR*	6.2000E-12	X E(-E/KT)	PIPER, SETSER, CLYNE, JCP 63, 4018 (1975)
45	KRF* + AR + M + ARKR* + M	6.0000E-32		AVCO
46	KRF* + KR + M + KR2F* + M	5.0000E-31		AVCO
47	ARF* + AR + M + AR2F* + M	4.0000E-31		AVCO
48	ARF* + KR + M + ARKR* + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
49	AR2* + KR + AR + AR + KR*	8.0000E-11		ZAMIR (PRIV. COMMUN. TO SRI)
50	AR2* + AR2* + AR2(*) + AR + AR + E	3.0000E-10		E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
51	ARF* + KR + KRF* + AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
52	AR2* + F + ARF* + AR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
53	KR2* + F + KRF* + KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
54	AR2* + F2 + AR2F* + F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
55	ARKR* + F2 + KRF* + AR + F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976
56	ARKR* + F2 + ARKR* + F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
57	KR2* + F2 + KR2F* + F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
58	AR2F* + F2 + AR + AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
59	ARKRF* + F2 + AR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
60	KR2F* + F2 + KR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976

Fig. 4.9: Continued

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIGIK,1) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE 1TH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
61	ARKRF • KR • KR2F • AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
62	KRF • F2 • KR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
63	ARF • F2 • AR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
64	AR2F • KR • KRF • AR • AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
65	AR • M • AR • M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
66	KR • M • KR • M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
67	ARF • AR • F	3.3000E-07		SRI REPORT NO. MP 76-99, DEC., 1976
68	AR2 • AR • AR	3.0000E-06		SRI REPORT NO. MP 76-99, DEC., 1976
69	ARKR • AR • KR	3.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
70	KR2 • KR • KR	3.3000E-06		SRI REPORT NO. MP 76-99, DEC., 1976
71	AR2F • AR • AR • F	2.0000E-08		SRI REPORT NO. MP 76-99, DEC., 1976
72	ARKRF • AR • KR • F	5.0000E-07		SRI REPORT NO. MP 76-99, DEC., 1976
73	KR2F • KR • KR • F	6.7000E-07		SRI REPORT NO. MP 76-99, DEC., 1976
74	KRF • KR • F • HNU	1.1000E-08		R. BURNHAM, S. S. SEARLES (SUBMITTED TO JCP)
75	KRF • RAD • KR • F • RAD	2.0000E-16		LASER TRANSITION: STIMULATED EMISSION X-SECTION
76	F2 • RAD • F • F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
77	F • RAD • F • E	5.4000E-18		A. MANOL, PHYS REV A3, 291 (1971)
78	KR2F • RAD • AR • KR • F	1.0000E-99		CROSS SECTION UNKNOWN
79	AR2(•) • RAD • AR • AR(•)	1.5000E-17		STEVENS (PARK CITY CONFERENCE)
80	KR2(•) • RAD • KR • KR(•)	3.5000E-18		J. WEST (NRTC)

Fig. 4.9: Continued



CROSS SECTION (UNITS OF  $1.000E-16$  CM<sup>2</sup>) VS ELECTRON ENERGY (EV) FOR  
MOMENTUM TRANSFER FOR KR

REFERENCE -- FROST, PHELPS: KIEFFER REPT., P. 15

U (EV)	SIGMA(U) ( $1.0E-16$ CM <sup>2</sup> )
-----	
0.000	3.070E+01
.010	2.600E+01
.020	1.967E+01
.030	1.600E+01
.050	1.143E+01
.070	9.000E+00
.100	6.800E+00
.130	5.330E+00
.160	3.970E+00
.200	2.470E+00
.240	1.620E+00
.280	1.130E+00
.320	8.700E-01
.360	7.270E-01
.400	6.200E-01
.470	5.400E-01
.560	5.000E-01
.700	5.000E-01
.840	5.400E-01
1.000	6.170E-01
1.300	8.670E-01
1.600	1.320E+00
2.200	2.530E+00
3.000	4.840E+00
5.000	1.020E+01
7.000	1.500E+01
10.000	1.930E+01
12.000	2.200E+01
20.000	1.800E+01
23.000	1.500E+01
30.000	1.000E+01
40.000	5.000E+00
-----	

(DATA WAS SUBMITTED ON 03/01/77)

Fig. 4.10: Tabular summary of electron cross section data.

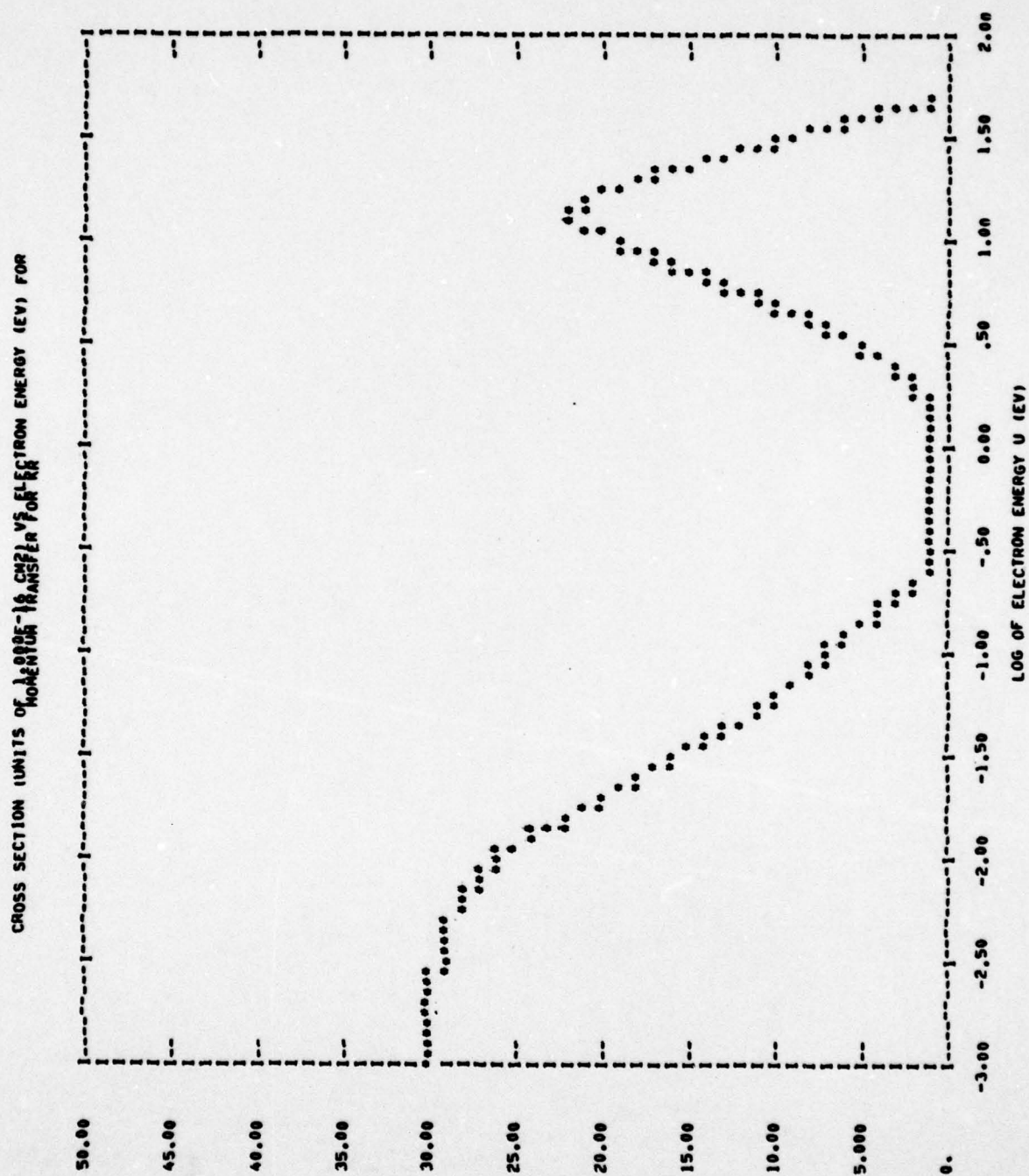


Fig. 4.11: Plot of electron cross section data.

```

TIME T = 2.000E-07 SEC
GAS MIXTURE --
AR /KR /F2 = 89.90 / 10.00 / .10
PLASMA PARAMETERS
-----
E (FIELD) = 8.3123E+02 VOLT/CM
TMOL = 300. DEG K
NMOL = 4.8893E+19 CM-3
PTOT = 1520.0 TORR
      = 2.00 ATM

E/N = 1.7001E-17 VOLT CM2
E/P = .55 V/CM/TORR
      = .42 KV/CM/ATM

<U> = 3.087 EV
TE = 2<U>/3K = 23889. DEG K

DIFFUSION D = 2131.97 CM2/SEC
MOBILITY MU = 646.9 CM2/VOLT/S
EK = D/MU = 3.296 EV
VDRIFT = MU*E = 5.3772E+05 CM/SEC

CONDUCT/NE = 1.0363E-16 CM2/Ohm
CONDUCT = 2.5572E-02 /Ohm-CM
RHO*NE = 9.6495E+15 Ohm/CM2
J/NE = E*VD = 8.6142E-14 AMP CM/EL

DISCHARGE = 1.7669E+04 WATT/CM3
DEPOSITION = 4.1411E+04 WATT/CM3
TOTAL POWER = 5.9080E+04 WATT/CM3

INELASTIC = 4.4363E+04 WATT/CM3
ELASTIC HEAT = 1.4642E+04 WATT/CM3
E<U>DNE/DT = 3.6592E+02 WATT/CM3
POWER DISS = 5.9371E+04 WATT/CM3

NU(NOM) = 2.8272E+12 SEC-1
NE = 2.4676E+14 CM-3
NE/NMOL = 5.0468E-06
S(U = 0)/NE = 9.6958E+06 SEC-1
S(U > 0)/NE = 1.0476E+08 SEC-1
NU(IONIZE) = 2.0009E+07 SEC-1
NU(ATT.REC) = 1.3146E+08 SEC-1
DNE/DT/NE = 2.9988E+06 SEC-1
DNE/DT = 7.3996E+20 CM-3/SEC
-----

CALCULATION PARAMETERS USED:
MESH = 500. EMAX = 20.00 EV. DE = .040 EV.

```

Fig. 4.12: Summary of plasma parameters.



NORMALIZED ELECTRON DISTRIBUTION FUNCTION  $F(U)$ , IN UNITS OF  $\text{EV}^{3/2}(-3/2)$ , WITH OUTPUT AT  $\sim 200$  FV INTERVALS. THE ELECTRON ENERGY RANGE 10, 20,001 EV WAS SUBDIVIDED INTO 500 INTERVALS, GIVING A RESOLUTION  $\sim .040$  EV.

E/NTOT = 1.70E-17 VOLT CM2 = .547 VOLT/CM/TORR = .416 KVOLT/CM/ATM  
FRACTIONAL IONIZATION = NE/NTOT = 5.047E-06, NE = 2.468E-14 CM-3  
AR /KR /F2 = 89.90 / 10.00 / .10, TMOL = 300. DEG K

U (eV)	F (U)	U (eV)	F (U)	U (eV)	F (U)	U (eV)	F (U)	U (eV)	F (U)
0.000	2.37257E-01	.200	2.26004E-01	.400	2.25926E-01	.600	2.21737E-01	.800	2.14309E-01
1.000	2.04710E-01	1.200	1.94431E-01	1.400	1.83417E-01	1.600	1.72206E-01	1.800	1.61055E-01
2.000	1.50173E-01	2.200	1.39645E-01	2.400	1.29552E-01	2.600	1.19355E-01	2.800	1.10014E-01
3.000	1.02190E-01	3.200	9.40991E-02	3.400	8.65108E-02	3.600	7.94000E-02	3.800	7.27663E-02
4.000	6.65624E-02	4.200	6.07721E-02	4.400	5.53767E-02	4.600	5.03507E-02	4.800	4.56974E-02
5.000	4.13012E-02	5.200	3.74050E-02	5.400	3.37552E-02	5.600	3.04001E-02	5.800	2.73422E-02
6.000	2.45369E-02	6.200	2.19739E-02	6.400	1.96351E-02	6.600	1.75025E-02	6.800	1.55594E-02
7.000	1.37900E-02	7.200	1.21776E-02	7.400	1.07070E-02	7.600	9.37284E-03	7.800	8.16036E-03
8.000	7.00600E-03	8.200	6.12156E-03	8.400	5.26789E-03	8.600	4.51402E-03	8.800	3.85005E-03
9.000	3.26076E-03	9.200	2.75064E-03	9.400	2.31220E-03	9.600	1.92192E-03	9.800	1.58102E-03
10.000	1.20370E-03	10.200	1.03001E-03	10.400	8.20006E-04	10.600	6.40637E-04	10.800	5.07101E-04
11.000	3.91099E-04	11.200	2.96601E-04	11.400	2.19007E-04	11.600	1.58013E-04	11.800	1.11797E-04
12.000	7.06320E-05	12.200	5.60006E-05	12.400	4.00031E-05	12.600	3.07529E-05	12.800	2.40076E-05
13.000	1.97079E-05	13.200	1.60346E-05	13.400	1.47107E-05	13.600	1.29000E-05	13.800	1.13009E-05
14.000	9.93301E-06	14.200	8.72439E-06	14.400	7.65515E-06	14.600	6.71722E-06	14.800	5.90540E-06
15.000	5.41339E-06	15.200	4.97300E-06	15.400	4.60246E-06	15.600	4.26121E-06	15.800	3.90950E-06
16.000	3.52906E-06	16.200	3.17339E-06	16.400	2.85057E-06	16.600	2.58305E-06	16.800	2.34151E-06
17.000	2.12760E-06	17.200	1.93594E-06	17.400	1.76904E-06	17.600	1.62412E-06	17.800	1.49760E-06
18.000	1.30639E-06	18.200	1.20709E-06	18.400	1.20051E-06	18.600	1.12201E-06	18.800	1.05335E-06
19.000	9.90760E-07	19.200	9.33093E-07	19.400	8.82202E-07	19.600	8.3521E-07	19.800	7.62625E-07
20.000	3.10267E-07								

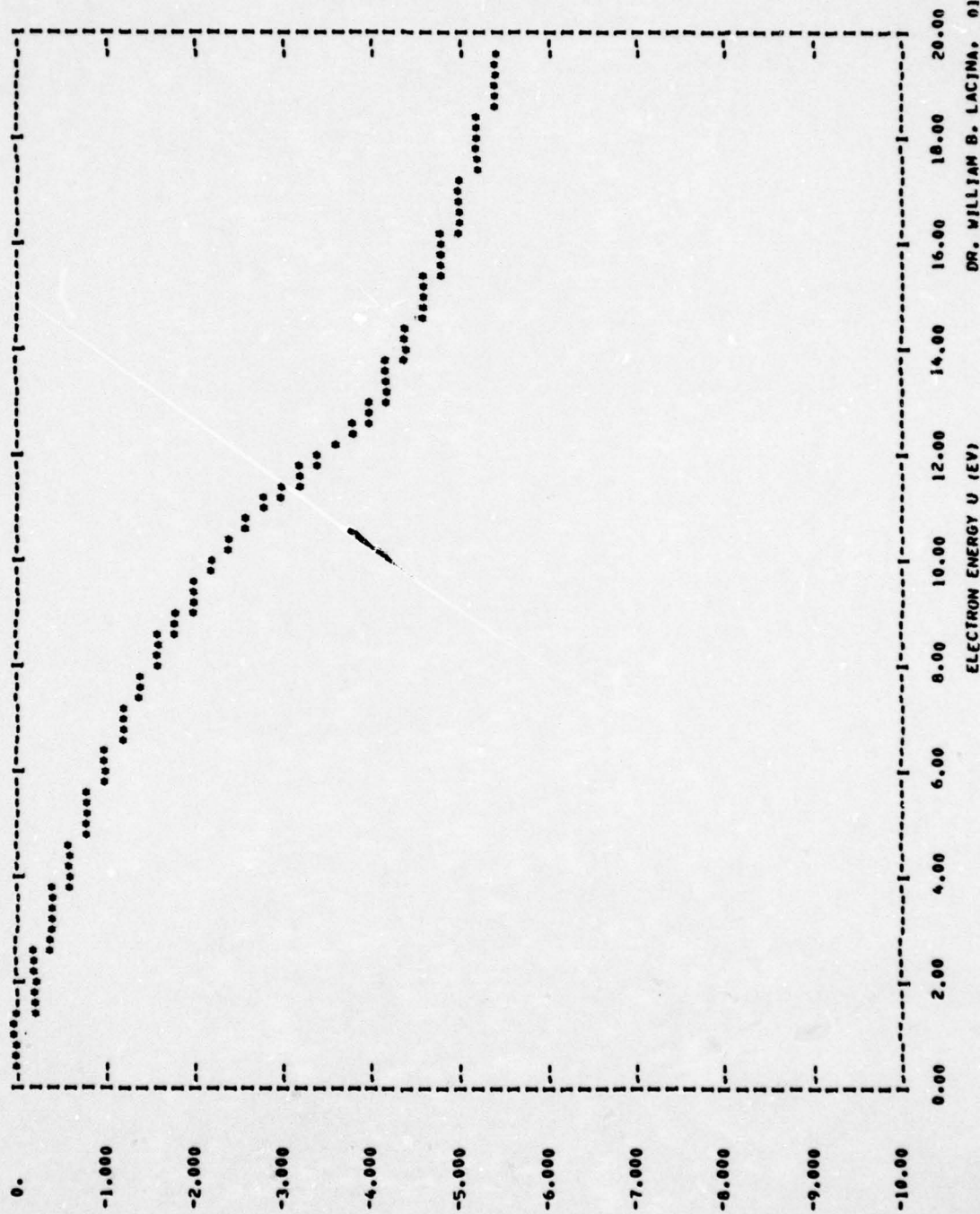
F(U) CONVERGED IN 1.0 SEC. IN 12 ITERATIONS! MAXIMUM RELATIVE CHANGE IN LAST ITERATION < 4.530E-04! POWER BALANCE ACCURACY = .20 %.

DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

**Fig. 4.13: Tabular electron distribution.**

LOG PLOT OF ELECTRON DISTRIBUTION  $F(U)/F(0)$  AS A FUNCTION OF ELECTRON ENERGY  $U$  (EV), WHERE  $F(0) = 2.373E-01$  EV\*\*(-3/2)

$E/NTOT = 1.709E-17$  VOLT CM<sup>2</sup> = .547 VOLT/CM/TORR = .416 KVOLT/CM/ATH  
 FRACTIONAL IONIZATION = NE/NTOT = 5.847E-06, NE = 2.468E+14 CM-3  
 AR /KR /F2 = 89.90 / 10.00 / .10, THOL = 300. DEG K

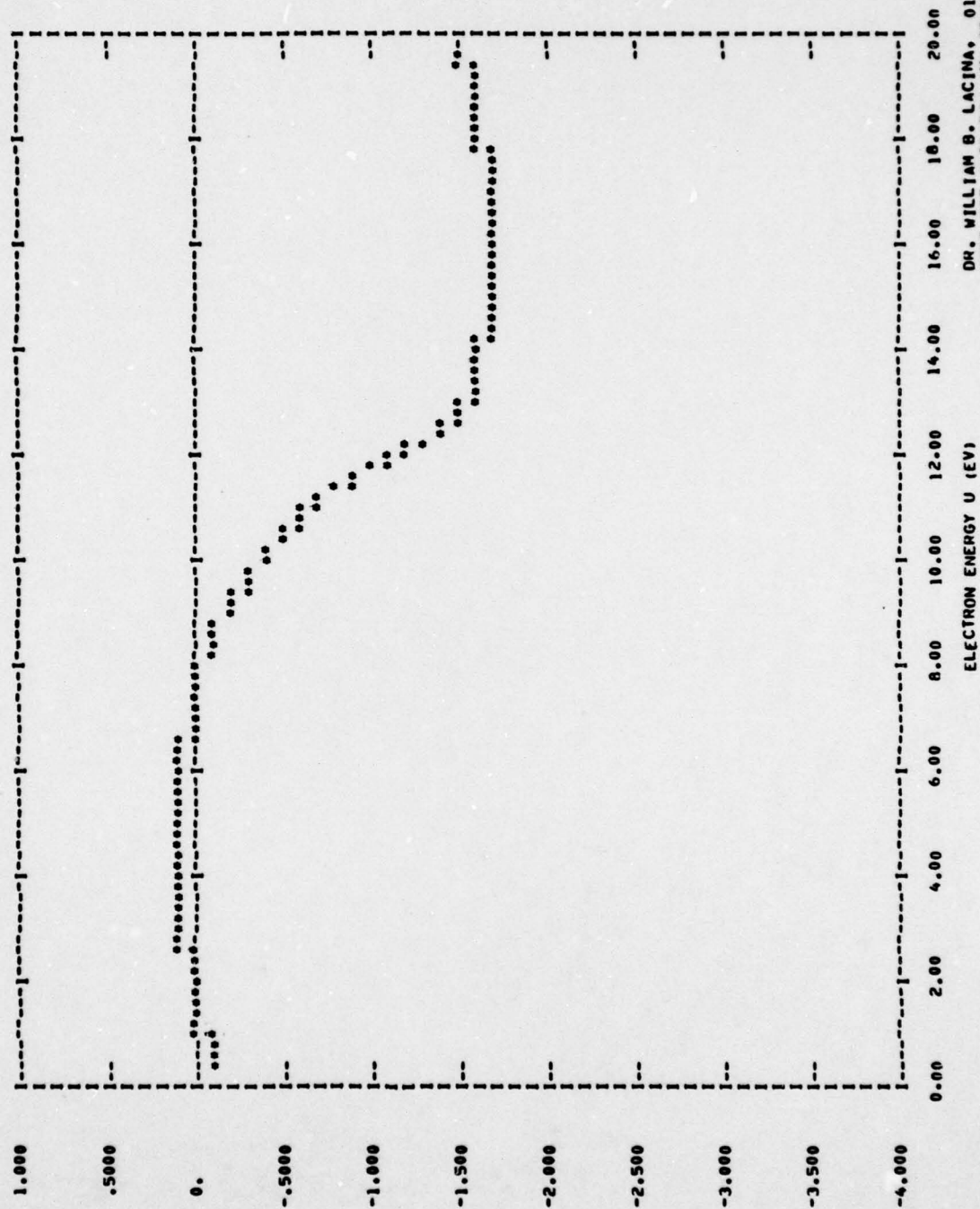


DR. WILLIAM B. LACINA, 01/12/79  
 NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.14: Plot of electron distribution function.

LOG PLOT OF RELATIVE ELECTRON DISTRIBUTION FUNCTION  $F(U)/F_{BOLTZ}(U, T_E)$ , WHERE  $T_E = (2/3)U_{AVG}/K_B = 23889$ , DEG K

$E/NTOT = 1.700E-17$  VOLT CM<sup>2</sup> = .547 VOLT/CM/TORR = .416 KVOLT/CM/ATM  
 FRACTIONAL IONIZATION =  $NE/NTOT = 5.047E-06$ ,  $NE = 2.468E+14$  CM<sup>-3</sup>  
 $AR/KR/F2 = 89.90 / 10.00 / .10$ ,  $THOL = 300$ , DEG K



DR. WILLIAM B. LACINA, 01/12/79  
 NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.15: Plot of electron distribution, normalized to Maxwellian.



TIME T = 2.000E-07 SEC

PLASMA KINETICS ANALYSIS WITH SUMMARY OF ELECTRON PARAMETERS, COLLISION RATES,  
AND POWER BALANCE FOR ALL ELASTIC AND INELASTIC COLLISION PROCESSES INCLUDED

E/NTOT = 1.708E-17 VOLT CM2 = .547 VOLT/CM/TORR = .416 KVOLT/CM/ATM  
FRACTIONAL IONIZATION = NE/NTOT = 5.047E-06, NE = 2.468E+14 CM-3  
AR /KR /F2 = 89.90 / 10.00 / .10, TMOL = 300. DEG K

U(AVG) = 3.087 EV, TE = 23889. DEG K, VD = 5.38E+05 CM/SEC, MU = 6.47E+02 CM2/VOLT/SEC

J	REACTION(J)	N(A) (CM-3)	N(B) (CM-3)	U(I) (EV)	DNE/DT/NE (SEC-1)	<V>S(G(A+B)) (CM3/SEC)	<V>S(G(B-A)) (CM3/SEC)	(NET) POWER PERCENT (WATT/CM3 ) POWER
1	AR + E → AR* + E	4.395E+19	1.582E+14	11.50		7.084E-13	7.610E-09	1.464E+04 24.78
2	KR + E → KR* + E	4.888E+18	2.528E+14	9.90		4.542E-12	9.396E-09	1.361E+04 23.03
3	AR + E → AR** + E	4.395E+19	3.331E+12	13.50		2.244E-14	7.606E-10	7.759E+03 13.13
4	KR + E → KR** + E	4.888E+18	5.876E+12	11.50		5.612E-14	7.028E-10	5.250E+02 .89
5	AR* + E → AR** + E	1.582E+14	3.331E+12	2.00		4.402E-07	1.079E-06	1.228E+02 .21
6	KR* + E → KR** + E	2.528E+14	5.876E+12	1.60		4.908E-07	9.900E-07	5.221E+03 8.84
7	AR + E → AR(+) + E + E	4.395E+19		15.80	6.771E+06	1.540E-13		7.480E-03 12.66
8	KR + E → KR(+) + E + E	4.888E+18		14.40	2.952E+06	6.039E-13		4.229E+03 7.16
9	AR* + E → AR(+) + E + E	1.582E+14		4.30	3.176E+06	2.008E-08		1.680E+03 2.84
10	KR* + E → KR(+) + E + E	2.528E+14		4.50	5.858E+06	2.317E-08		5.398E+02 .91
11	AR** + E → AR(+) + E + E	3.331E+12		2.30	2.796E+05	8.394E-08		1.042E+03 1.76
12	KR** + E → KR(+) + E + E	5.876E+12		2.90	9.740E+05	1.658E-07		2.542E+01 .04
13	AR2(+) + E → AR* + AR	3.792E+12		-1.900E+05	5.010E-08			1.117E+02 .19
14	KR2(+) + E → KR* + KR	1.962E+14		-1.474E+07	7.516E-08			1.489E+01 .03
15	F2 + E → F + F-	3.915E+16		-1.165E+08	2.976E-09			1.155E+01 1.95
								8.490E+02 1.44

DISCHARGE POWER = 1.767E+04 WATT/CM3 29.91 %  
SOURCE DEPOSITION = 4.141E+04 WATT/CM3 70.09 %

TOTAL ELECTRICAL = 5.908E+04 WATT/CM3 100.00 %

F(U) CONVERGED IN 1.8 SEC IN 12 ITERATIONS! MAXIMUM RELATIVE CHANGE IN LAST ITERATION < 4.530E-04! POWER BALANCE ACCURACY = .20 %

POWER INTO INELASTIC E-MOLECULE COLLISIONS = 4.434E+04 75.09 %  
ELASTIC E-MOLECULE HEATING = 1.464E+04 24.78 %  
D/DT(STORED ELECTRON KINETIC ENERGY) = E<U>DNE/DT = 3.659E+02 .62 %  
E-E POWER TRANSFER DISCREPANCY = -1.713E+02 -.29 %  
TOTAL POWER INTO COLLISIONS, HEATING, STORAGE = 5.920E+04 100.20 %

DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.16: Tabular summary of collision rates and power partition.

POPULATION DENSITIES AND RATES OF CHANGE					ELECTRICAL AND OPTICAL PARAMETERS		
TIME T = 2.000E-07 SEC					PARAMETER	VALUE	UNITS
I	SPECIES NAME	E(I) (EV)	N(I) (CM-3)	DN(I)/DT (CM-3/SEC)	TAU(I) 1.0E-09 SEC		
1	RAD	.00	1.796E+14	-2.735E+20	656.69	JBEAM	= 9.00 AMP/CM2
2	E(-)	3.09	2.468E+14	7.400E+20	333.47	DEPOSITION	= 2.00 KEV
3	AR	0.00	4.395E+19	4.056E+20	1.08E+08	ENERGY	= 300. KV/CM
4	AR*	11.50	1.582E+14	-4.525E+20	349.58	DVIX	= 14.66 KV/CM3
5	KR	0.00	4.888E+18	-2.001E+20	2.44E+07	P(BEAM)	= 131.92 CM-3/SEC
6	KR*	9.90	2.528E+14	-1.321E+20	1913.65	S(U > 0)	= 2.585F+22 CM-3/SEC
7	AR**	13.50	3.331E+12	1.832E+20	18.19	S(U = 0)	= 2.393E+21 CM-3/SEC
8	KR**	11.50	5.876E+12	2.791E+20	21.06	AREA	= 2000.00 CM2
9	AR(+)	15.80	3.368E+13	-7.757E+19	436.81	DIST	= 10.00 CM
10	KR(+)	14.40	8.307E+13	-4.943E+19	1680.66	CONDUCT	= 2.557E-02 /OHM/CM
11	AR2(+)	13.00	3.792E+12	-4.756E+18	797.34	R(DISCH)	= 1.955E-01 OHM
12	KR2(+)	11.80	1.962E+14	1.936E+20	1013.36	Q	= 4.547E-02 COULOMB
13	F2	0.00	3.915E+16	-4.643E+22	843.25	I(DTISCH)	= 4.352E+04 AMP
14	F	0.00	1.922E+16	9.361E+22	205.31	J(DTISCH)	= 2.126E+01 AMP/CM2
15	F-	0.00	8.222E+13	-6.878E+20	119.54	ESUS	= .831 KVOLT/CM
16	AR2*	9.50	7.830E+12	-6.812E+18	1149.38	ESUS*JSUS	= 17.67 KV/CM3
17	KR2*	8.20	1.935E+14	-9.538E+19	2029.03	Q/C	= 45.467 KVOLT
18	ARKR(+)	12.40	1.208E+13	-9.677E+18	1248.25	V(DTISCH)	= 8.312 KVOLT
19	ARKR*	8.80	1.102E+13	5.240E+18	2102.31	L*01/DY	= 37.155 KVOLT
20	ARF*	6.50	4.525E+12	-9.489E+18	476.85	REFLECT	= 70.00 %
21	AR2F*	5.00	5.678E+12	-1.118E+19	507.71	LOSS	= 0.00 %/PASS
22	KRF*	5.00	2.832E+13	4.689E+18	4334.34	T(CAVITY)	= 24.3 NS
23	KR2F*	3.00	1.474E+14	-4.736E+19	3112.68	L(CAVITY)	= 130.00 CM
24	ARKRF*	4.00	5.603E+12	7.128E+17	8141.54	LENGTH	= 75.00 CM
INTEGRATION STEP SIZE = 2.619					OMEGA/4/PI	= 1.177E-04 CM-1	
ORDER OF INTEGRATION = 3					THRESH	= 2.378E-03 CM-1	
					NET GAIN	= 2.290E-03 CM-1	
					LASER GAIN	= 4.065E-03 CM-1	
					ABSORPTION	= 1.775E-03 CM-1	
					INTENSITY	= 4.316E+06 WATT/CM2	
					OPTICAL	= 10.26 KW/CM3	
					EFFICIENCY	= .01 %	
					E<U>ONE/DT	= 3.659F-01 KW/CM3	
					DE(TOT)/DT	= 9.371E-02 KW/CM3	
					E(TOT)	= 1.894F-03 J/CM3	
					HEAT * SP	= 1.392E+02 KW/CM3	
					DP(NEFORE)	= -.40 %	
					DP(AFTER)	= .06 %	

DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.17: Tabular summary of population densities and their rates of change (and effective time constants), electrical and optical parameters.



PERCENTAGE CONTRIBUTION OF REACTION K TO  $DN(I)/DT$ , EXPRESSED (FOR EACH SPECIES) AS A PERCENTAGE OF THE MAXIMUM RATE OCCURRING FOR ALL REACTIONS INCLUDED

K	RATE(K)	MAX %	RAD	E(-)	AR	AR*	KR	KR*	AR**	KR**	AR(-)	KR(-)
1	7.386E+21	45.3			-26.564	45.323						
2	4.892E+21	22.3					-22.339	16.765				
3	2.428E+20	1.5			-8.73				1.490			
4	6.666E+19	.3								.228		
5	1.630E+22	100.0				-100.000			100.000			
6	2.918E+22	100.0								100.000		
7	1.671E+21	7.8									7.794	4.079
8	7.283E+20	4.1										3.656
9	7.837E+20	4.8				-4.809						8.096
10	1.445E+21	8.1										.322
11	6.900E+19	.4										1.346
12	2.403E+20	1.3										
13	4.689E+19	.3										
14	3.638E+21	19.3			.169	.288						
15	2.875E+22	100.0					16.610	12.466				
16	1.932E+20	5.7			1.390							
17	4.776E+21	88.7					43.611					
18	2.143E+22	100.0			-77.087						100.000	
19	6.124E+21	37.6			-22.025	37.578						24.732
20	4.416E+21	24.7										
21	1.263E+21	5.8										
22	1.456E+22	100.0										
23	2.024E+21	10.7										
24	4.765E+21	26.7										
25	1.785E+22	100.0										
26	4.968E+21	27.8										
27	1.390E+22	100.0										
28	1.889E+22	100.0										
29	3.400E+21	100.0										
30	3.780E+20	7.0										
31	3.323E+21	61.7										
32	5.433E+21	100.0										
33	5.385E+21	100.0										
34	1.559E+20	3.4										
35	1.559E+20	4.0										
36	2.786E+21	60.0										
37	8.064E+21	42.7										
38	8.064E+21	81.6										
39	6.831E+21	38.3										
40	4.966E+20	2.6										
41	4.966E+20	17.5										
42	7.127E+21	32.5										
43	4.645E+21	100.0										
44	4.794E+21	29.4										
45	2.621E+21	92.4										
46	2.420E+21	24.6										
47	3.890E+21	100.0										
48	1.981E+20	3.8										
49	3.062E+21	90.1										
50	1.839E+16	.0										

Fig. 4.18: (Partial) reproduction of tabular summary of reaction sensitivities.

\* THIS REACTION CONTRIBUTES LESS THAN 5. % TO ALL SPECIES THROUGHOUT THE ENTIRE CALCULATION SO FAR



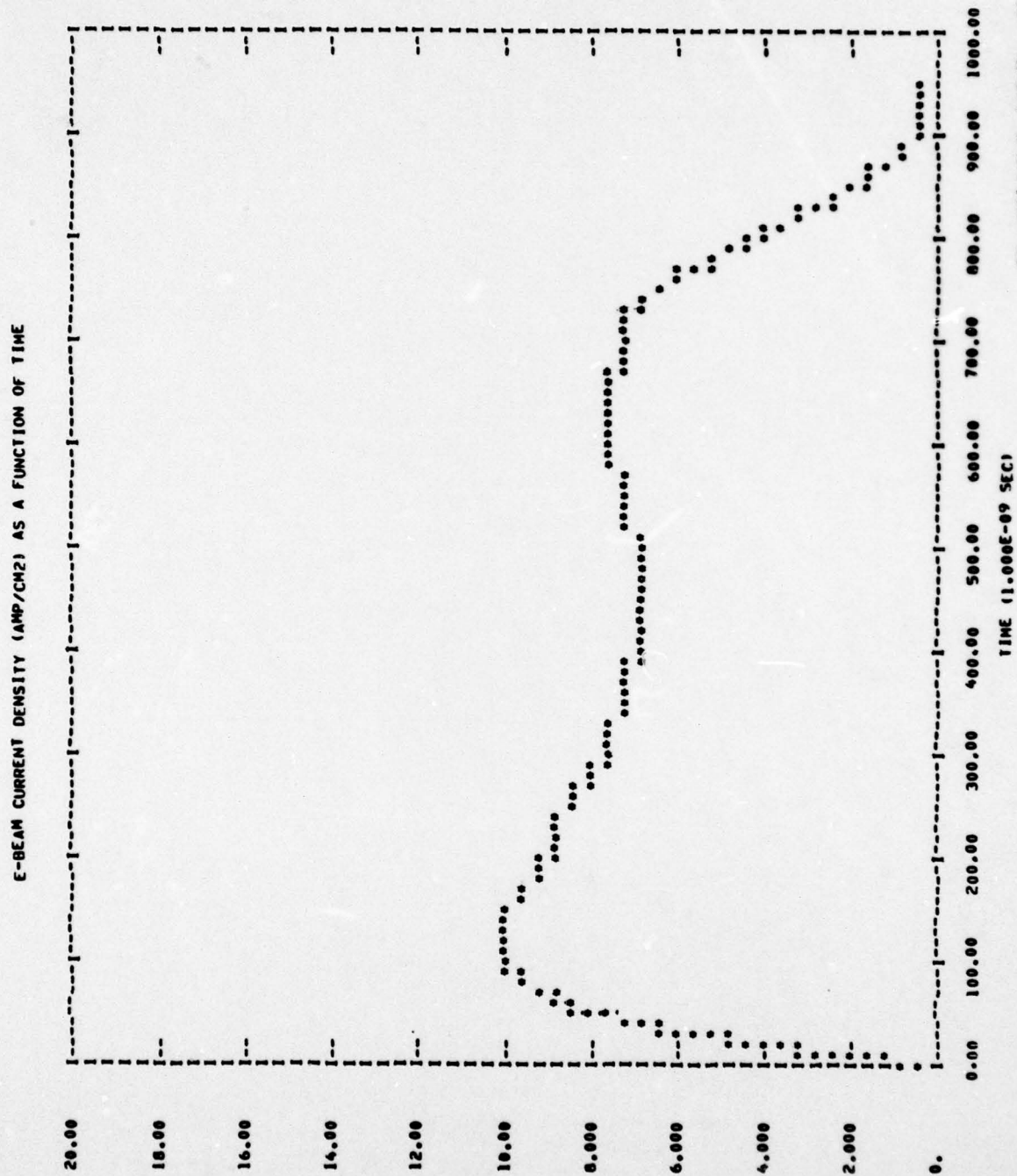
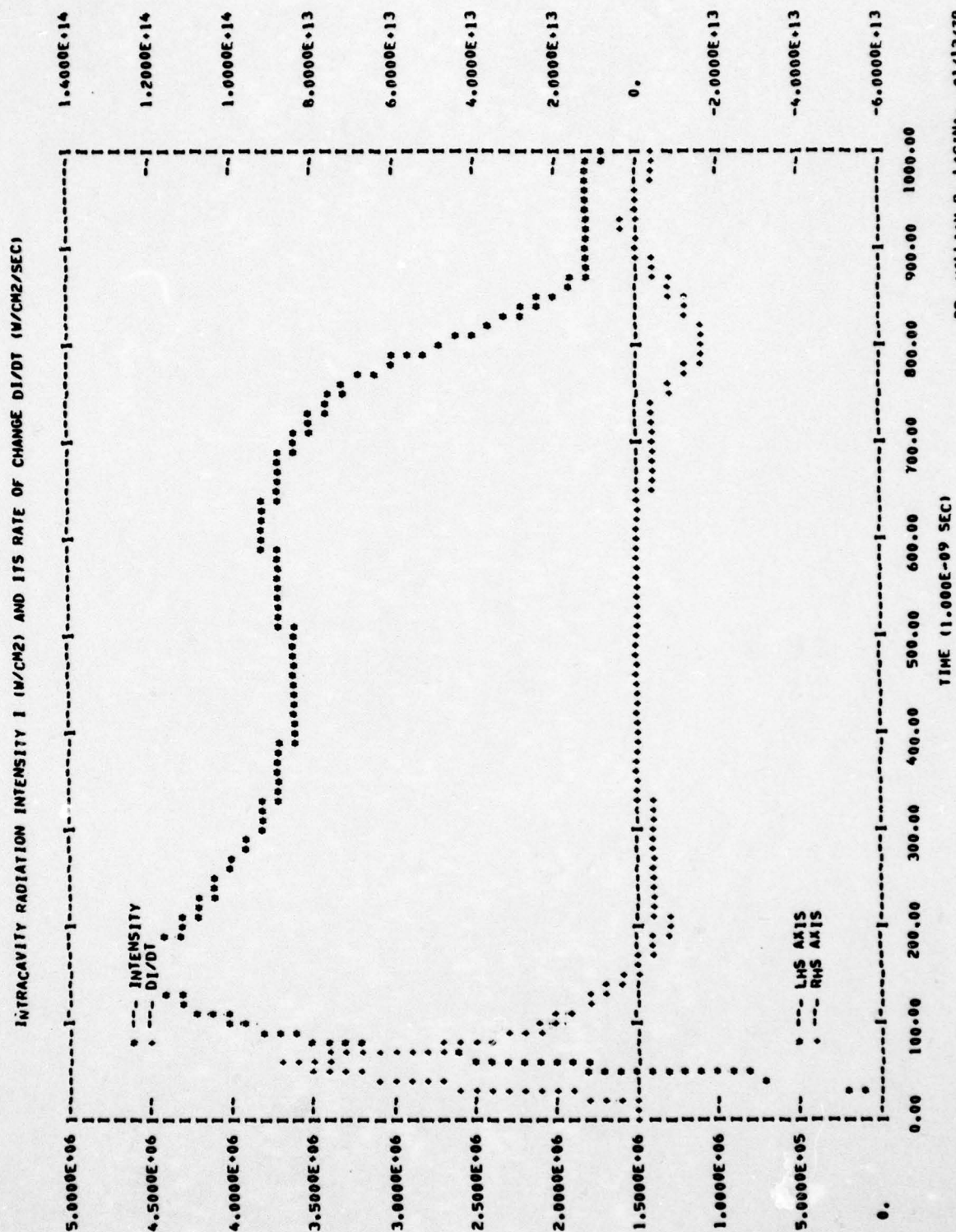


Fig. 4.19: Electron Beam current density as a function of time.



DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.20: Intracavity radiation intensity as a function of time.

SUMMARY OF ELECTRICAL AND OPTICAL PARAMETERS							
TIME (1.00E-09 SEC)	JBEAM (A/CN2)	PBEAM (KW/CN3)	VOLTAGE (KV)	JSUS (A/CN2)	DISCH (KW/CN3)	OUTPUT (KW/CN3)	OPT EFF (%)
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10.00	2.15	32.92	3.80	.08	.03	-.00	-.00
20.00	4.05	57.09	.39	4.00	.16	.00	.00
30.00	5.69	82.19	2.38	1.49	.35	.41	.50
40.00	7.07	102.29	3.36	4.75	1.60	4.16	4.00
50.00	8.20	119.09	3.31	5.52	1.83	9.74	8.06
60.00	8.70	126.63	3.53	6.93	2.45	10.45	8.10
70.00	9.14	133.05	3.77	8.11	3.05	10.29	7.56
80.00	9.50	138.35	4.02	9.31	3.74	10.26	7.22
90.00	9.78	142.57	4.28	10.46	4.48	10.42	7.08
100.00	10.00	145.72	4.53	11.57	5.25	10.64	7.05
110.00	10.08	146.90	4.81	12.63	6.08	10.82	7.07
120.00	10.12	147.51	5.12	13.65	6.98	10.92	7.07
130.00	10.12	147.56	5.43	14.67	7.97	10.96	7.05
140.00	10.08	147.03	5.76	15.68	9.03	10.96	7.03
150.00	10.00	145.93	6.10	16.67	10.17	10.92	6.99
160.00	9.76	142.52	6.50	17.56	11.41	10.77	7.00
170.00	9.54	139.43	6.95	18.42	12.80	10.53	6.91
180.00	9.34	136.64	7.41	19.35	14.34	10.28	6.81
190.00	9.16	134.14	7.87	20.31	15.99	10.07	6.70
200.00	9.00	131.92	8.31	21.26	17.67	9.88	6.61
210.00	8.92	130.92	8.72	22.23	19.38	9.75	6.49
220.00	8.84	129.71	9.07	23.22	21.06	9.69	6.42
230.00	8.74	128.32	9.41	24.09	22.67	9.64	6.38
240.00	8.62	126.76	9.75	24.93	24.31	9.57	6.34
250.00	8.50	125.02	10.10	25.73	26.00	9.49	6.29
260.00	8.31	122.28	10.49	26.47	27.76	9.38	6.25
270.00	8.13	119.80	10.90	27.16	29.62	9.23	6.18
280.00	7.97	117.54	11.33	27.92	31.63	9.09	6.09
290.00	7.83	115.51	11.73	28.72	33.68	8.96	6.01
300.00	7.70	113.69	12.09	29.50	35.65	8.88	5.94
310.00	7.62	112.57	12.40	30.28	37.54	8.82	5.88
320.00	7.54	111.43	12.66	31.05	39.30	8.80	5.84
330.00	7.46	110.28	12.88	31.74	40.88	8.79	5.82
340.00	7.38	109.13	13.09	32.36	42.37	8.78	5.79
350.00	7.30	107.98	13.30	32.99	43.86	8.75	5.76
360.00	7.20	106.59	13.50	33.55	45.30	8.72	5.74
370.00	7.12	105.32	13.71	34.09	46.75	8.68	5.71
380.00	7.04	104.17	13.91	34.66	48.22	8.64	5.67
390.00	6.96	103.13	14.09	35.22	49.61	8.61	5.64
400.00	6.90	102.19	14.23	35.76	50.90	8.59	5.61
410.00	6.83	101.14	14.36	36.26	52.07	8.57	5.60
420.00	6.77	100.32	14.47	36.73	53.15	8.55	5.57
430.00	6.73	99.73	14.56	37.21	54.17	8.53	5.54
440.00	6.71	99.37	14.61	37.70	55.07	8.53	5.52
450.00	6.70	99.24	14.60	38.20	55.78	8.54	5.51
460.00	6.73	99.69	14.54	38.70	56.26	8.56	5.49
470.00	6.77	100.18	14.42	39.16	56.49	8.61	5.49
480.00	6.81	100.73	14.28	39.55	56.48	8.65	5.50
490.00	6.85	101.33	14.13	39.88	56.36	8.69	5.51
500.00	6.90	102.00	13.98	40.19	56.20	8.72	5.51

Fig. 4.21: Tabular summary of miscellaneous electrical and optical parameters as a function of time (voltages, current, power densities).



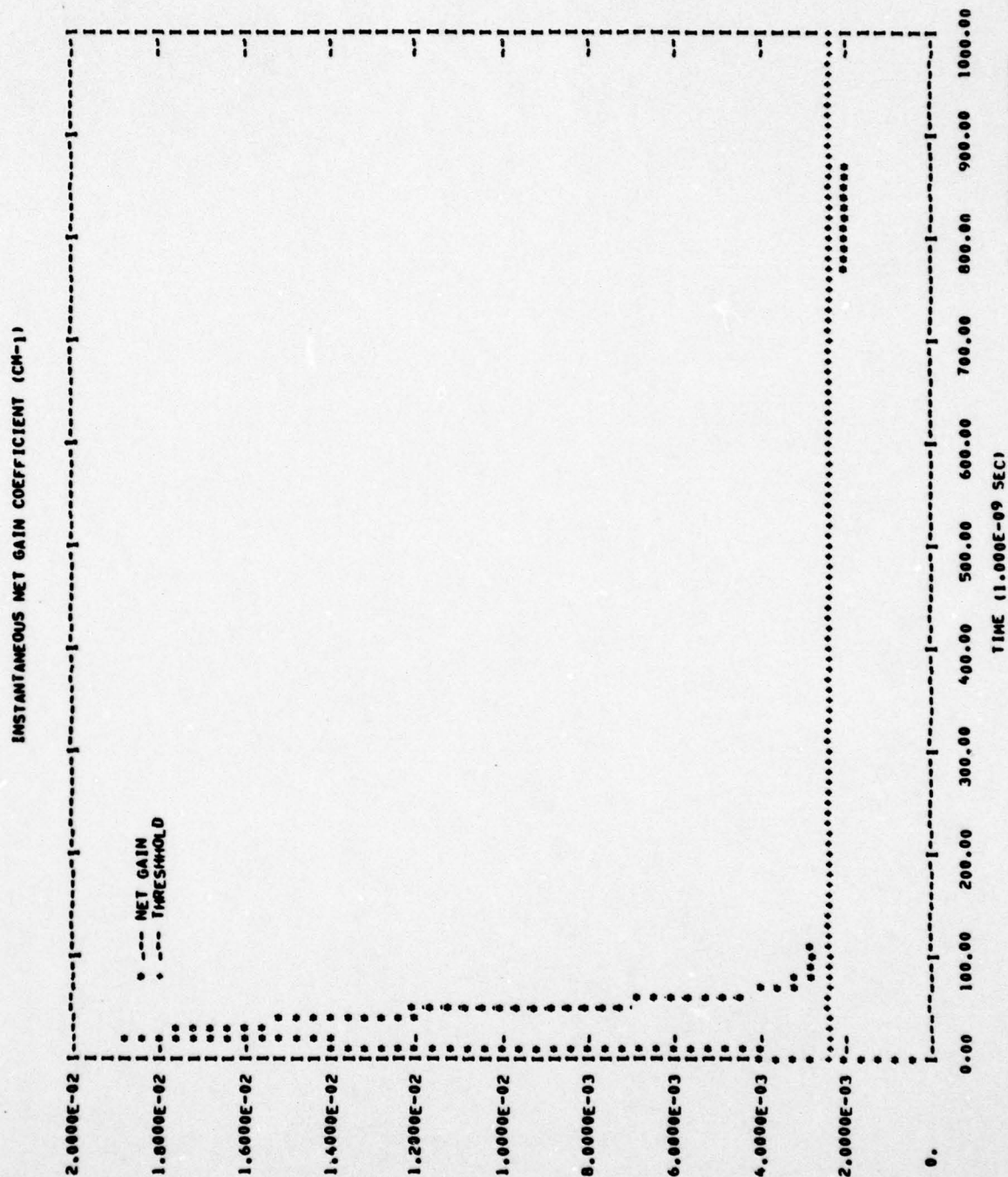
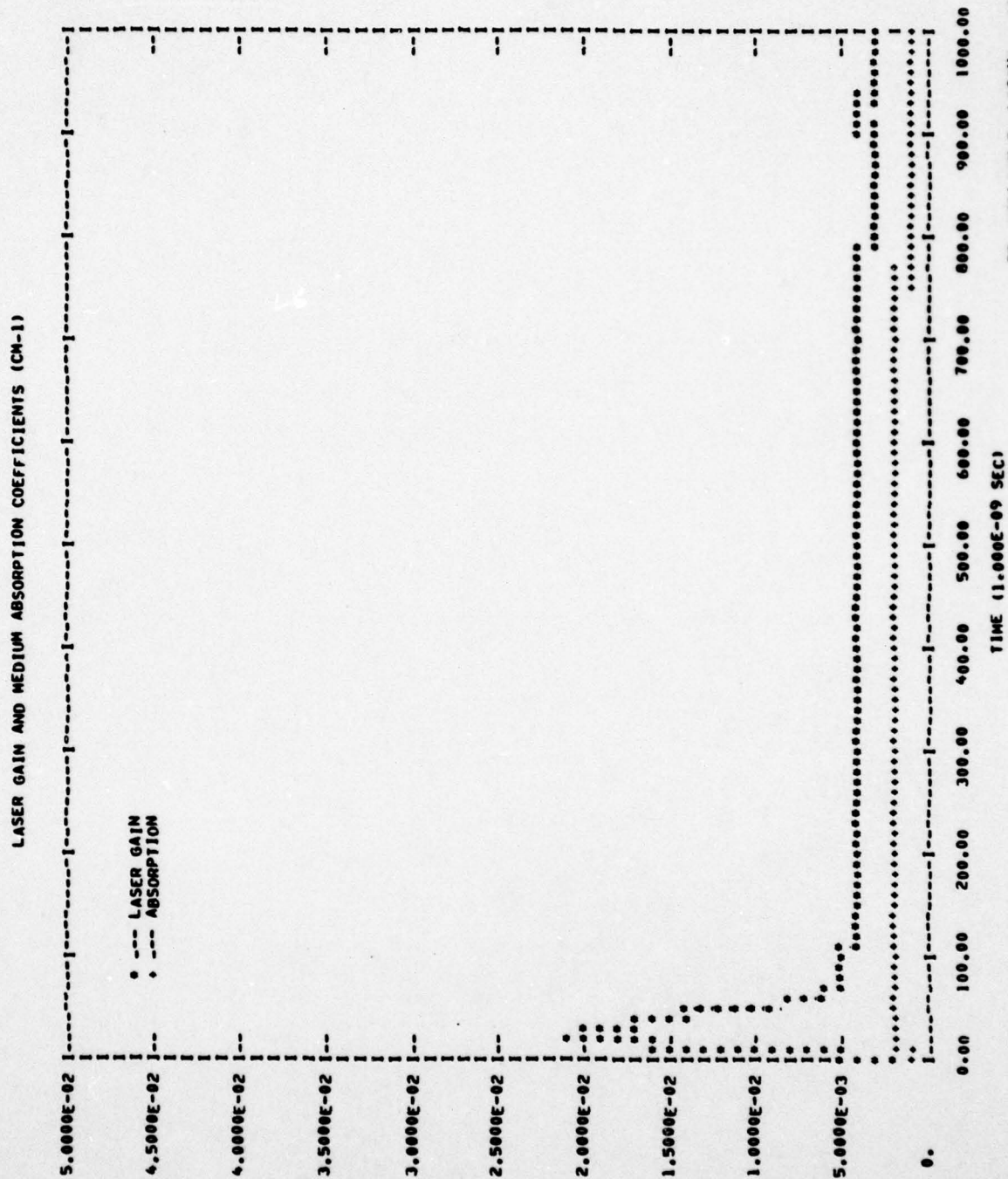


Fig. 4.22: Instantaneous net gain coefficient, relative to threshold, as a function of time.

DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY



DR. WILLIAM B. LACINA, 01/12/79  
 NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.23: Medium gain and absorption coefficients.

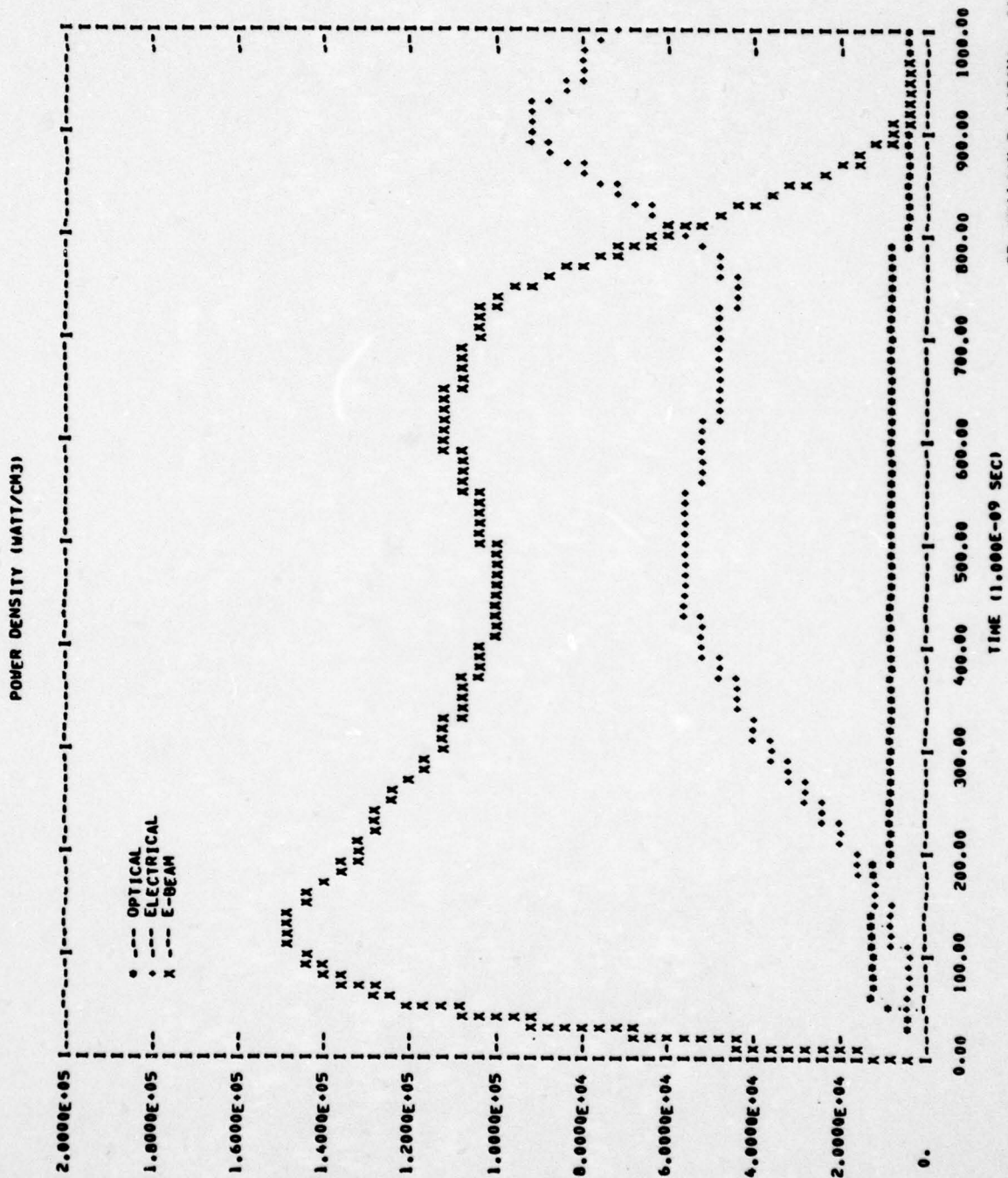


Fig. 4.24: Electrical and optical power densities.



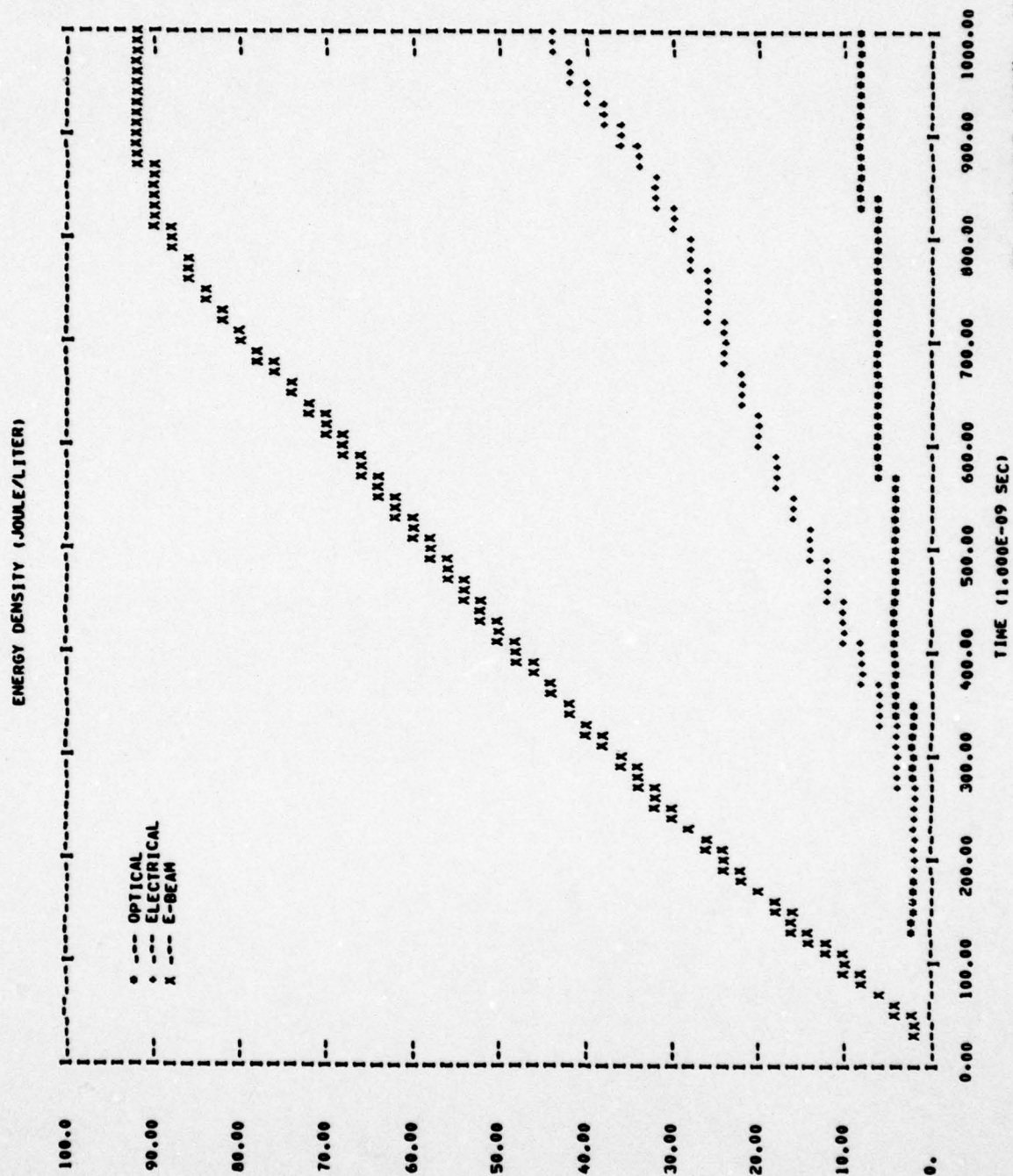
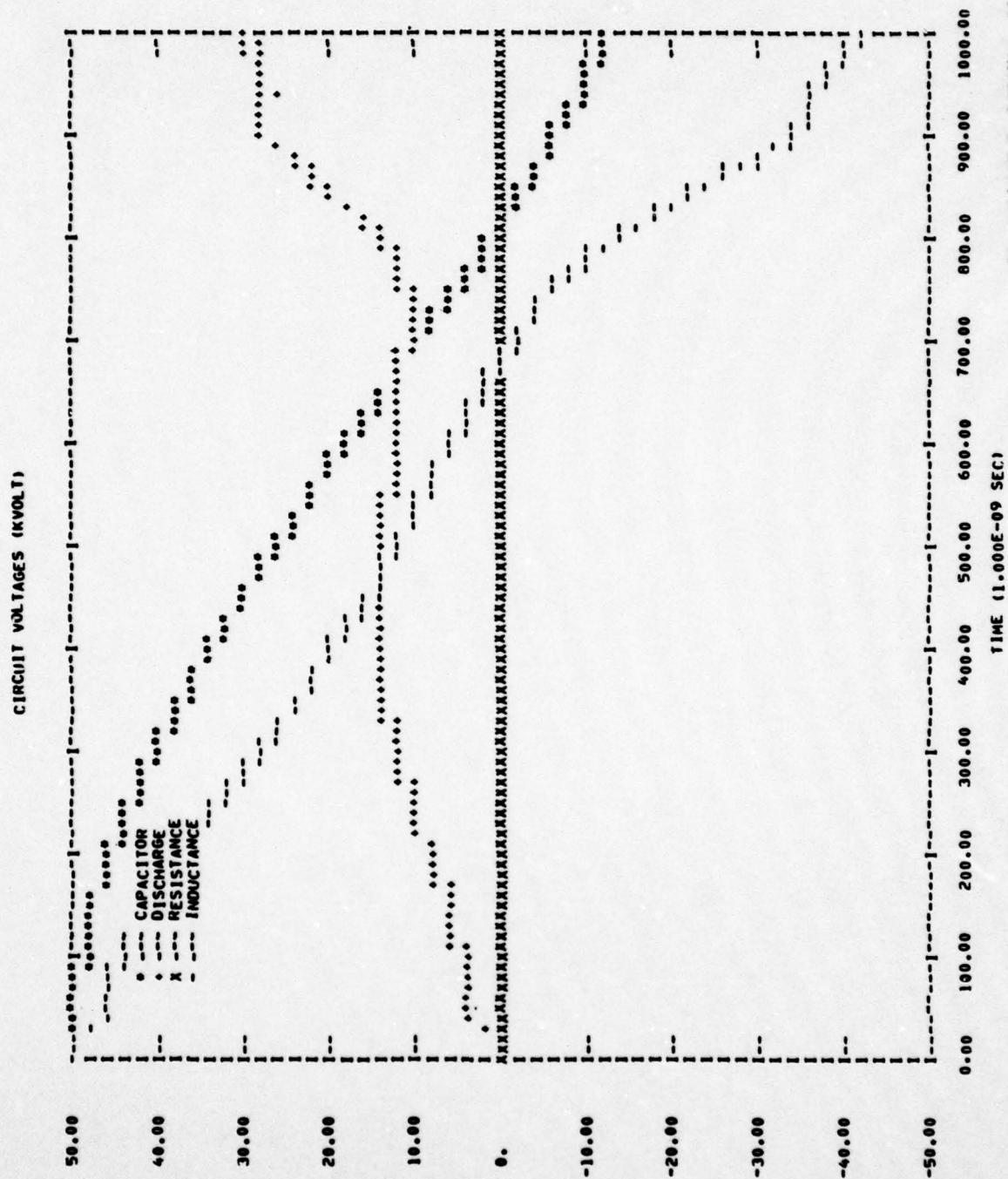
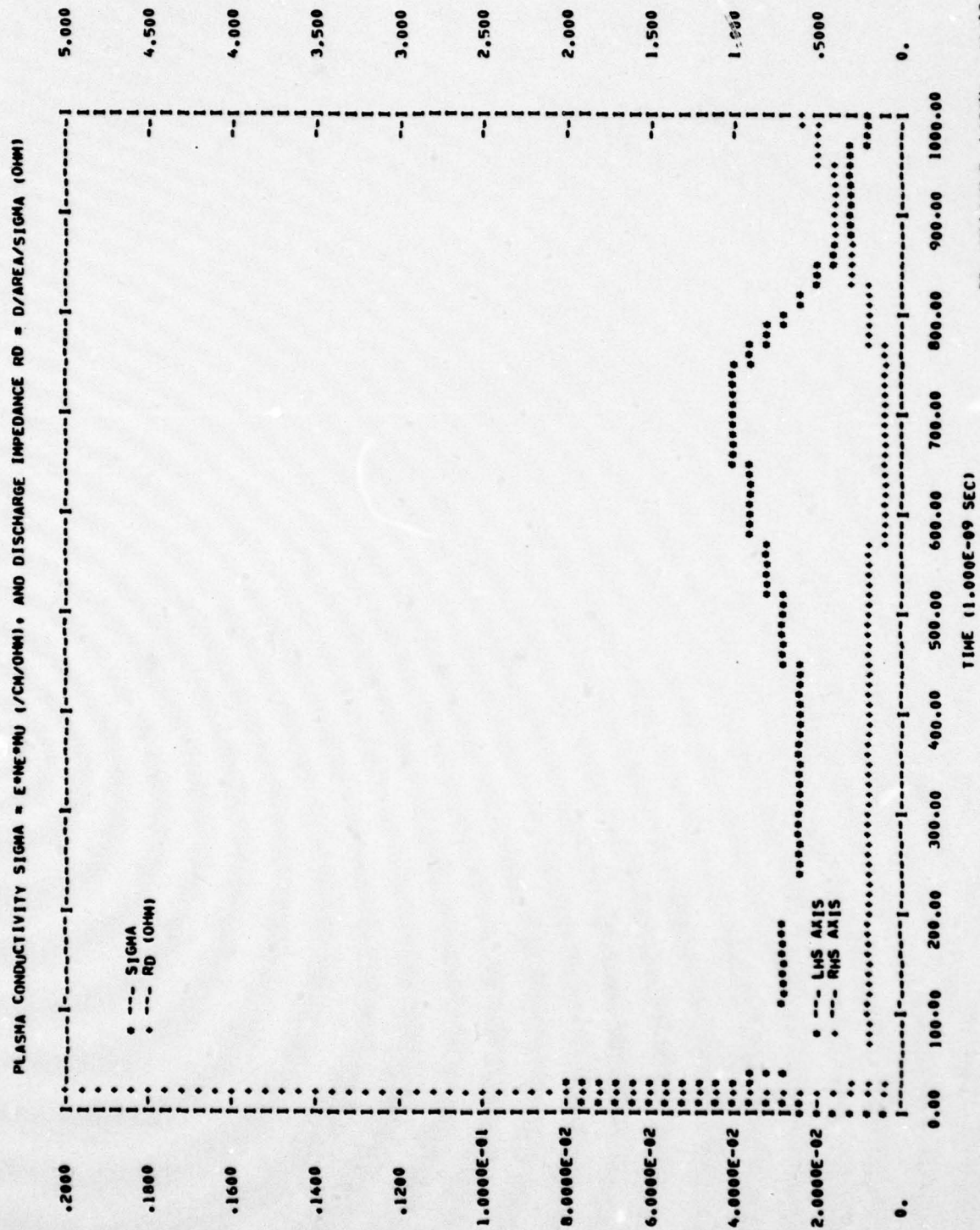


Fig. 4.25: Total (integrated) electrical and optical energy densities as a function of time.



DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

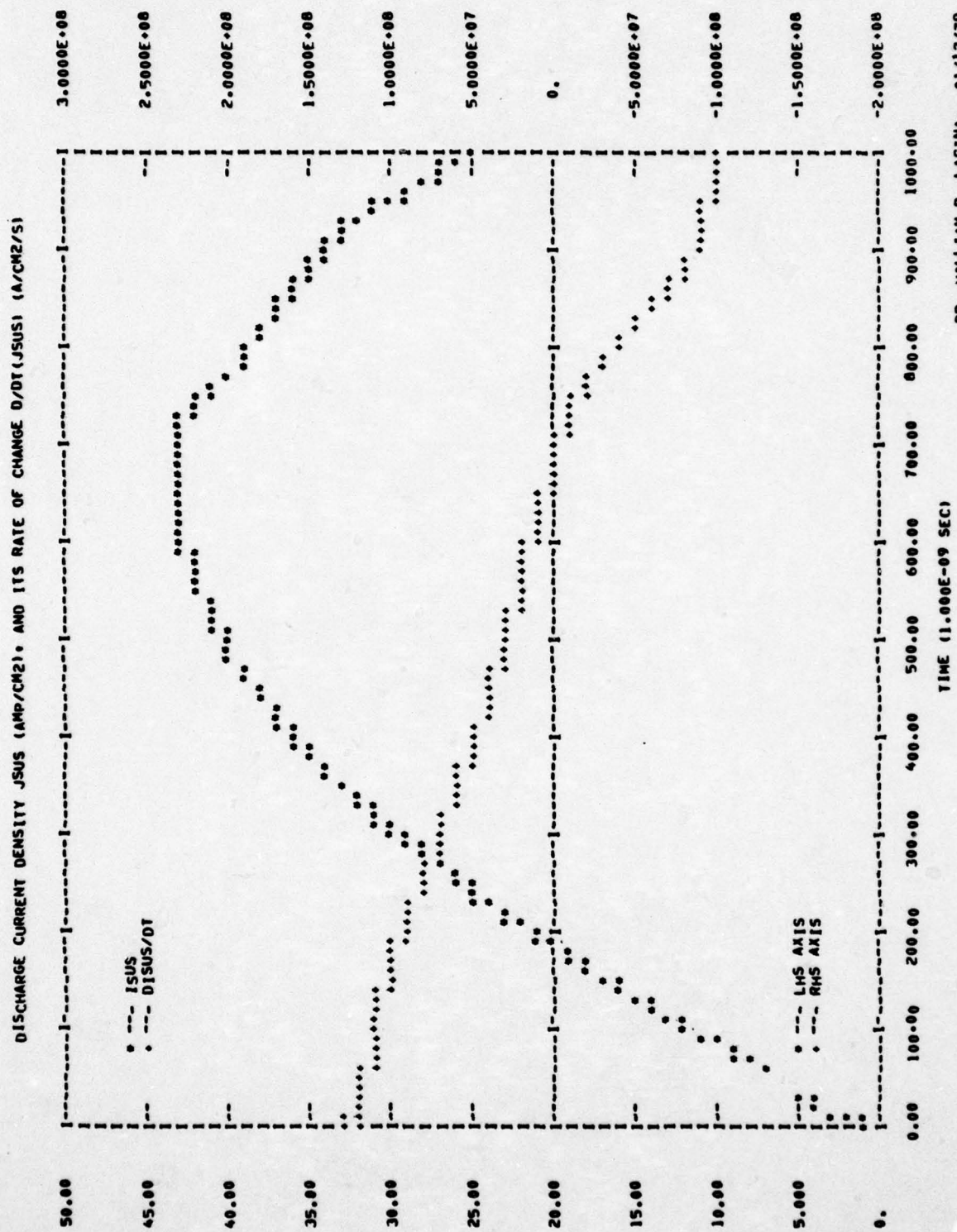
Fig. 4.26: Circuit voltages.



DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.27: Plasma conductivity and impedance.





DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.28: Discharge current density.

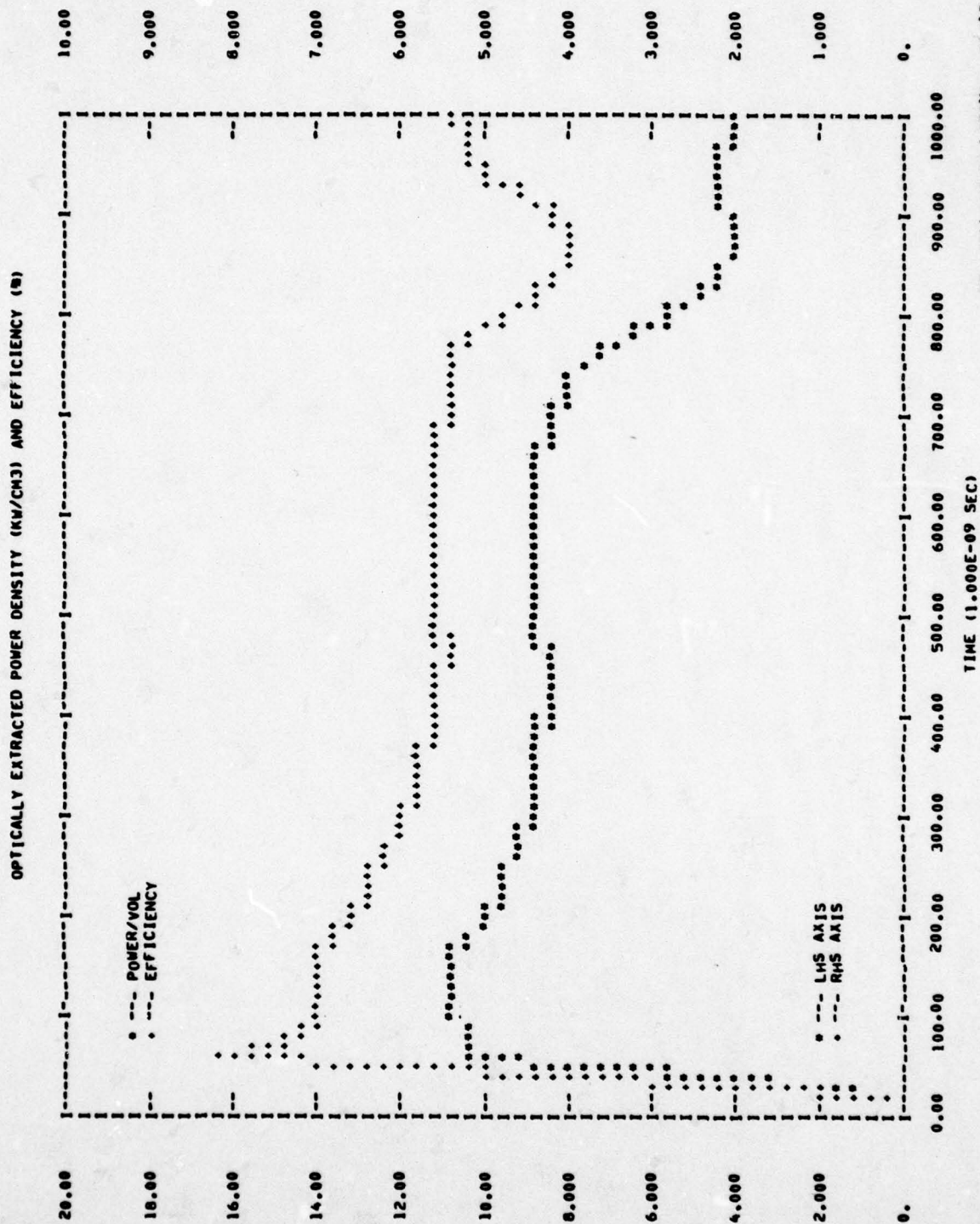
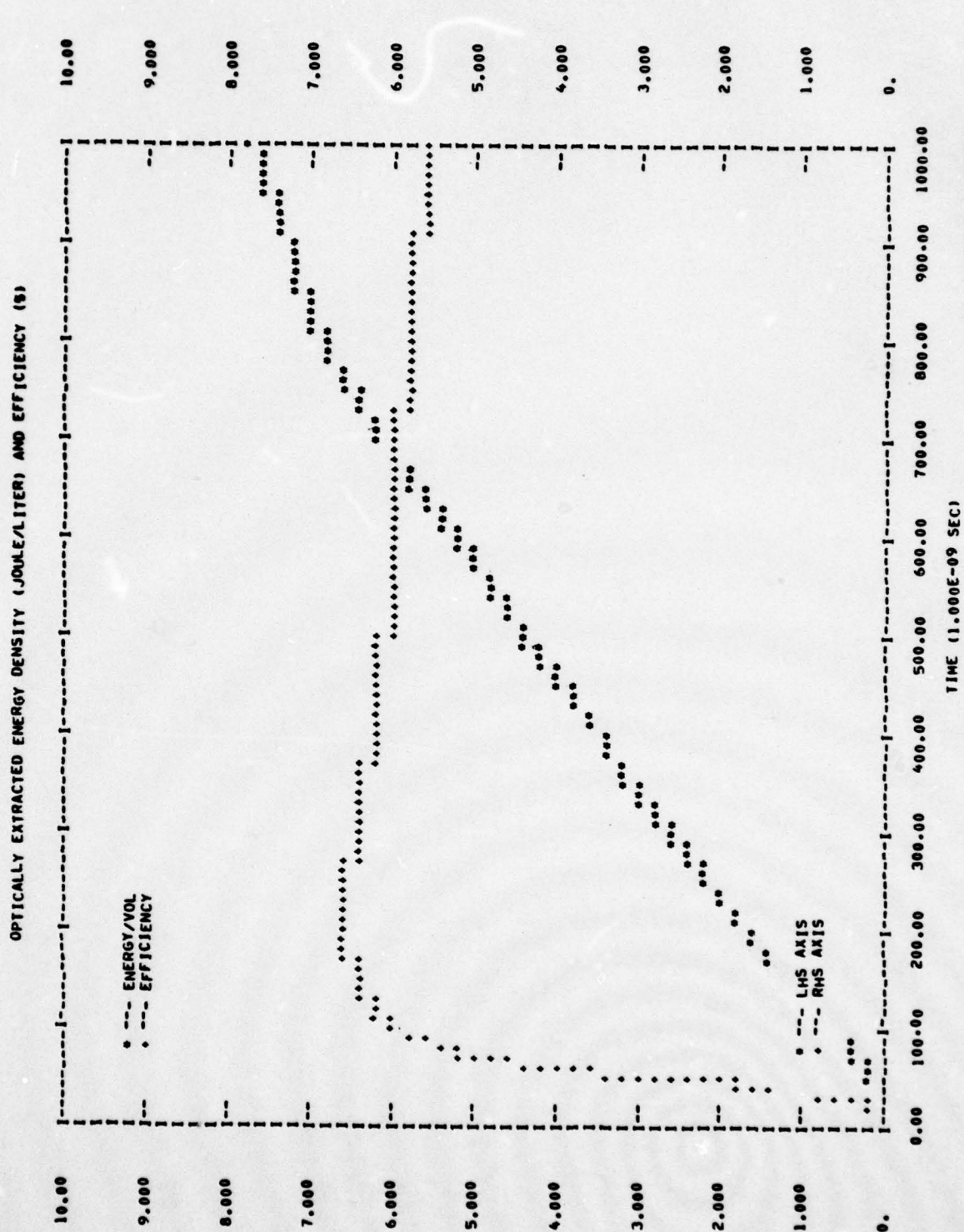


Fig. 4.29: Optically extracted power density, efficiency.

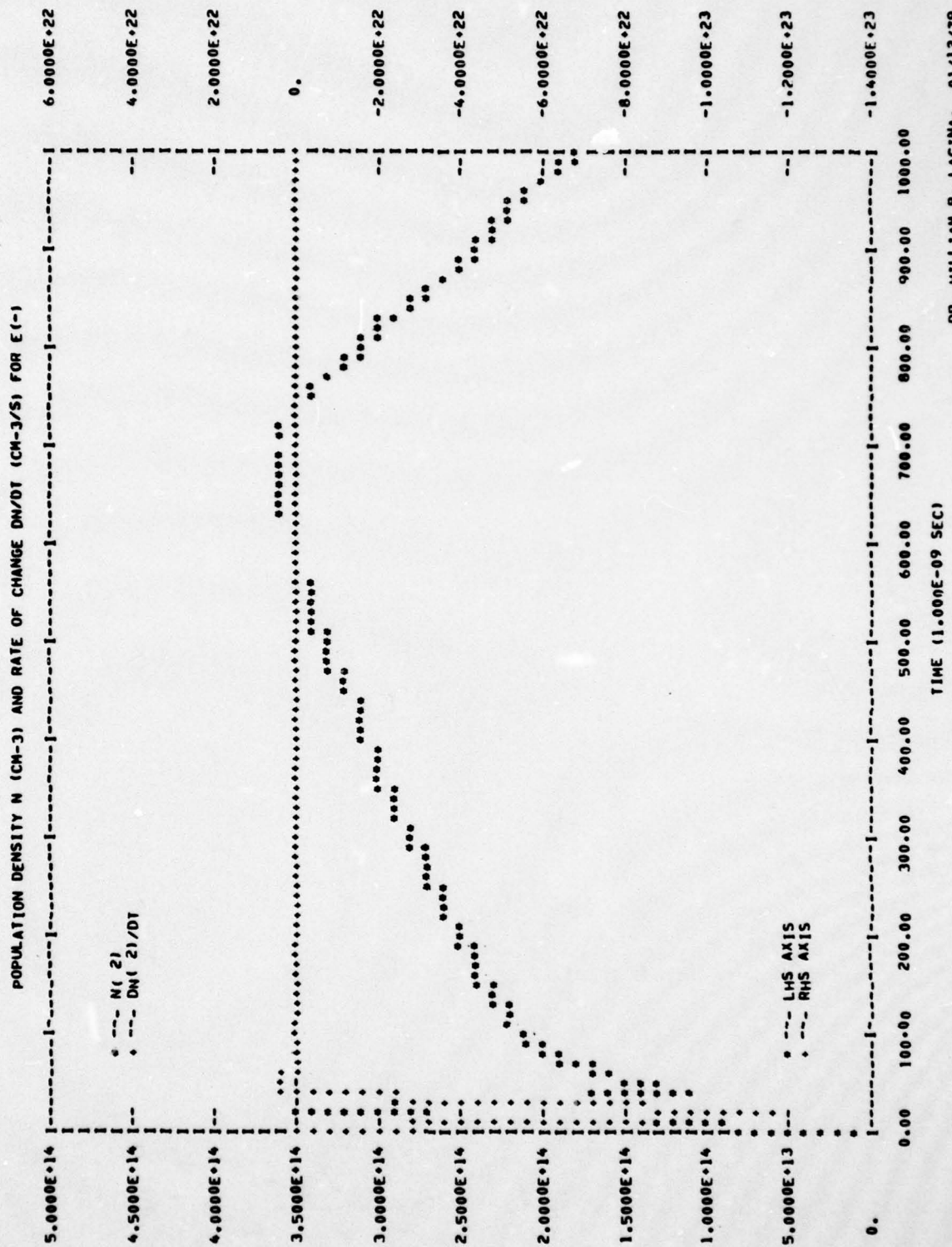
DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY



DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

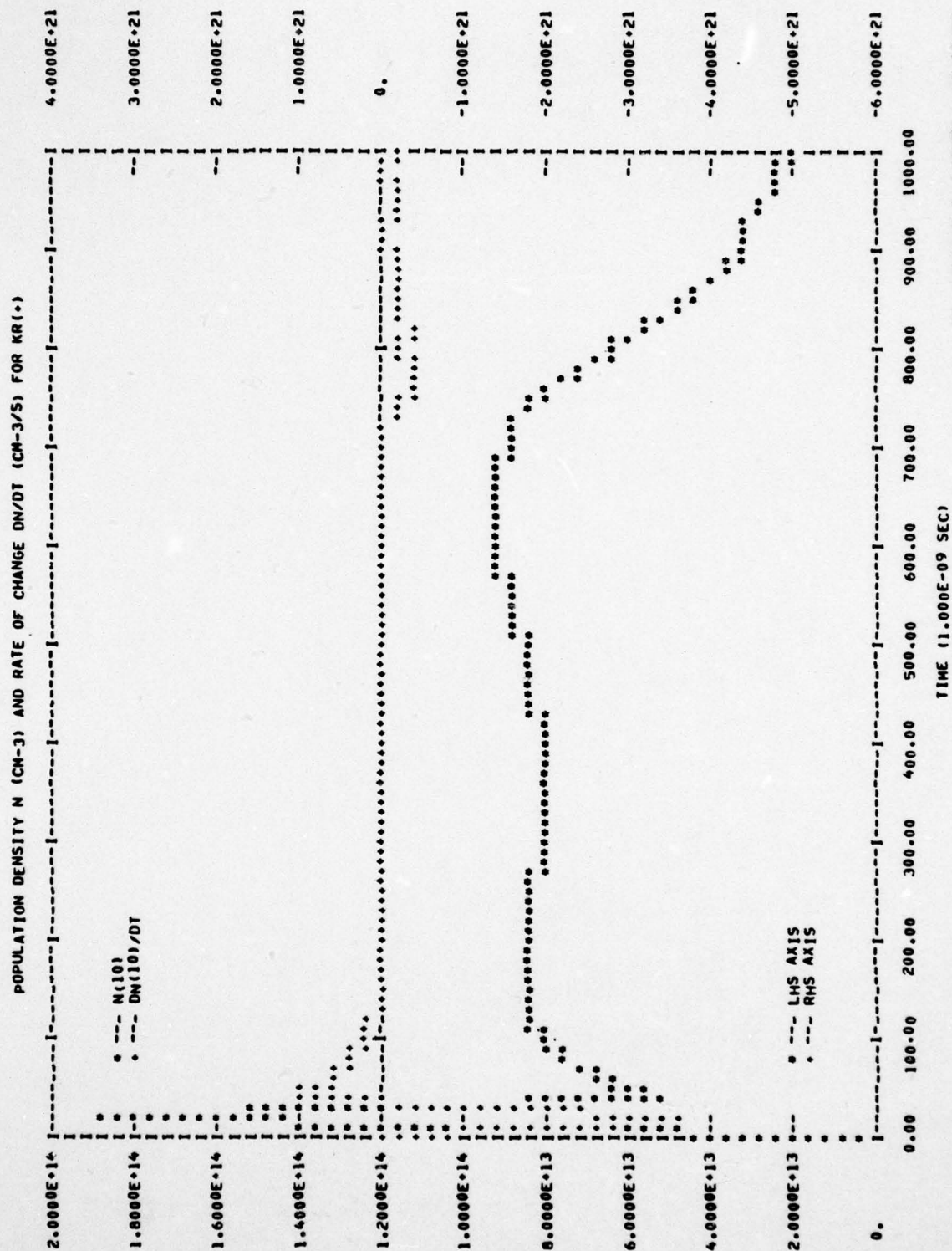
Fig. 4.30: Optically extracted energy density and efficiency.





DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.31: Population density and rate of change for e<sup>-</sup>.



DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.32: Population density and rate of change for  $Kr^+$ .

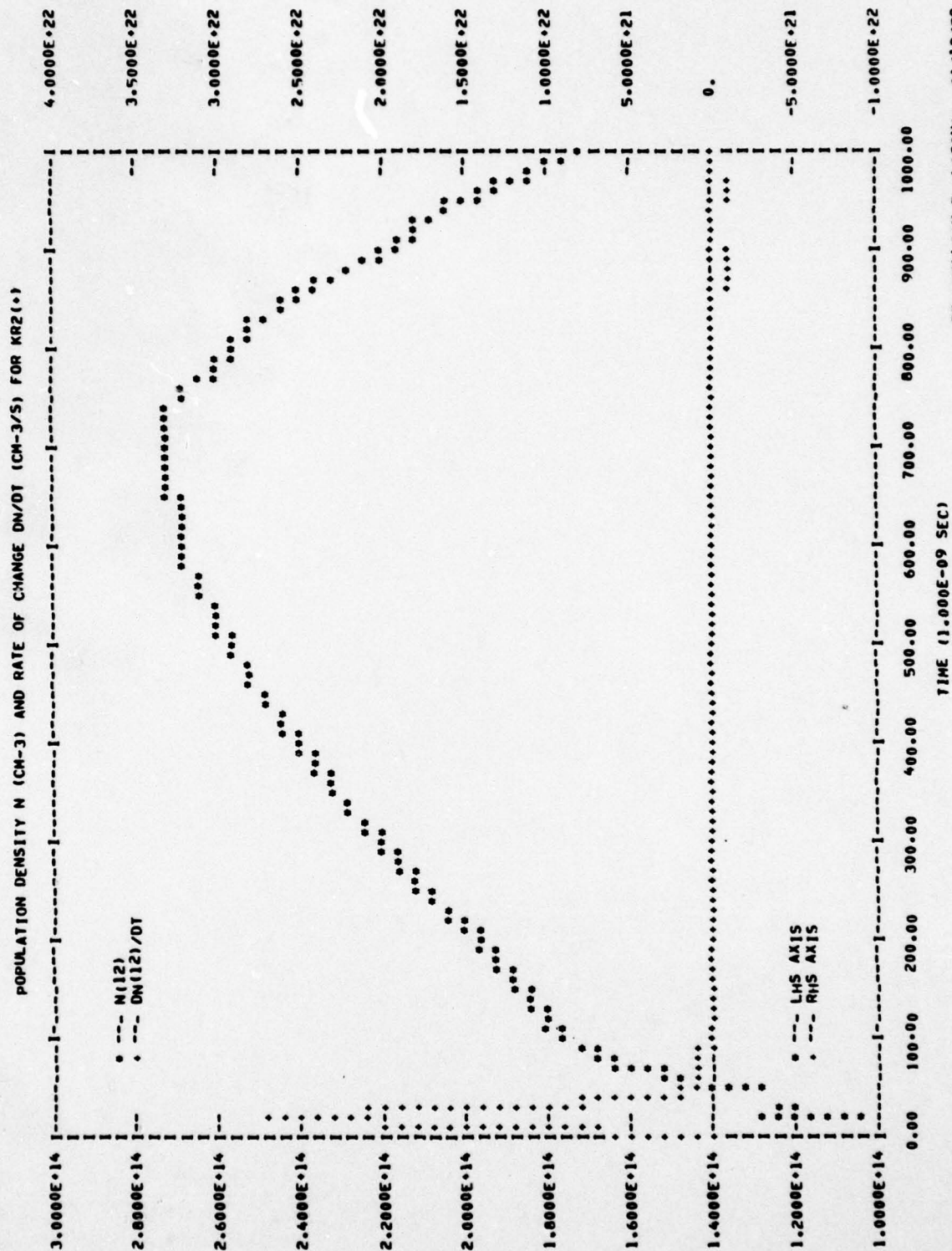
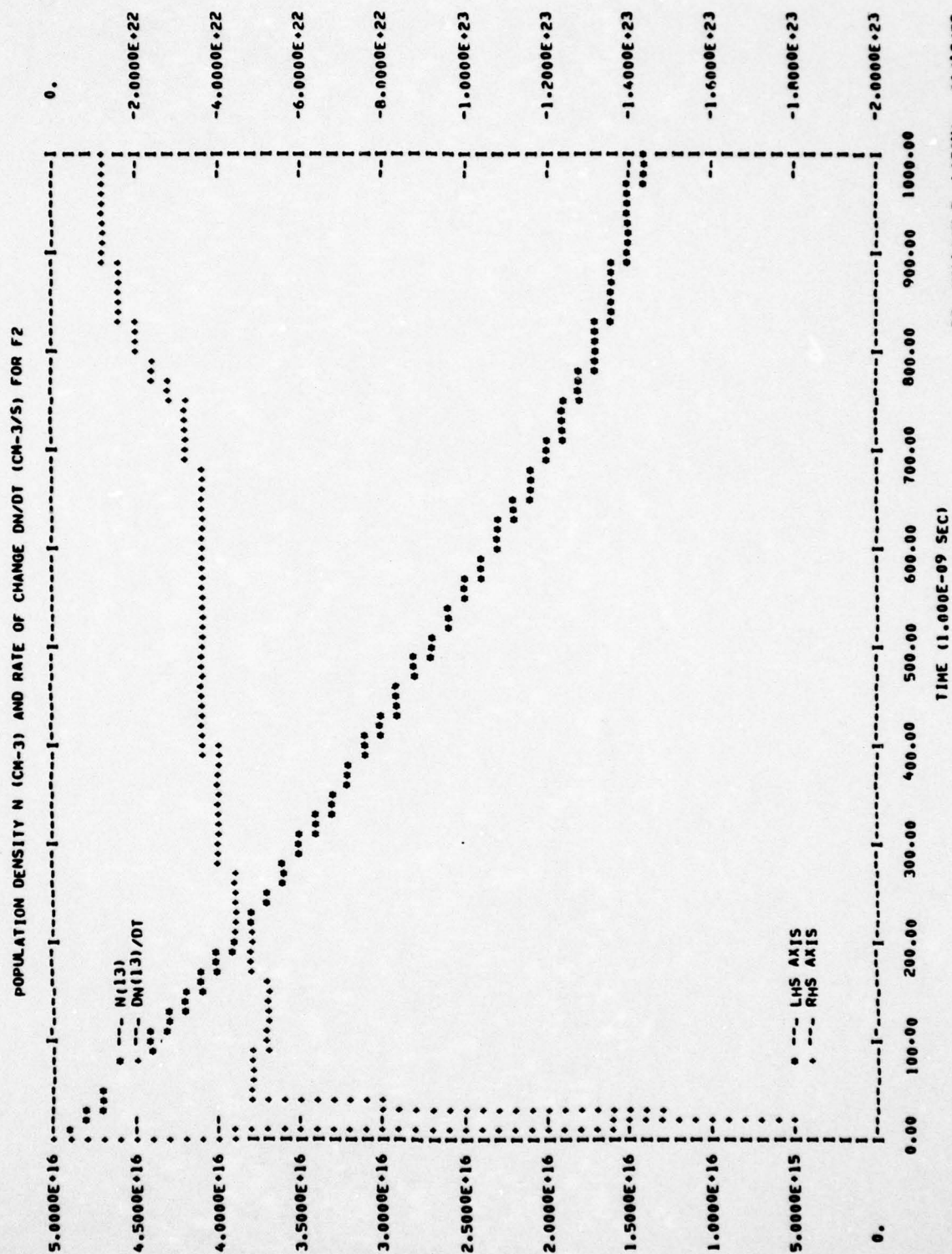


Fig. 4.33: Population density and rate of change for  $\text{Kr}_2^+$ .

DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY





DR. WILLIAM B. LACINA, 01/12/79  
NORTHROP RESEARCH AND TECHNOLOGY

Fig. 4.34: Population density and rate of change for F<sub>2</sub>.

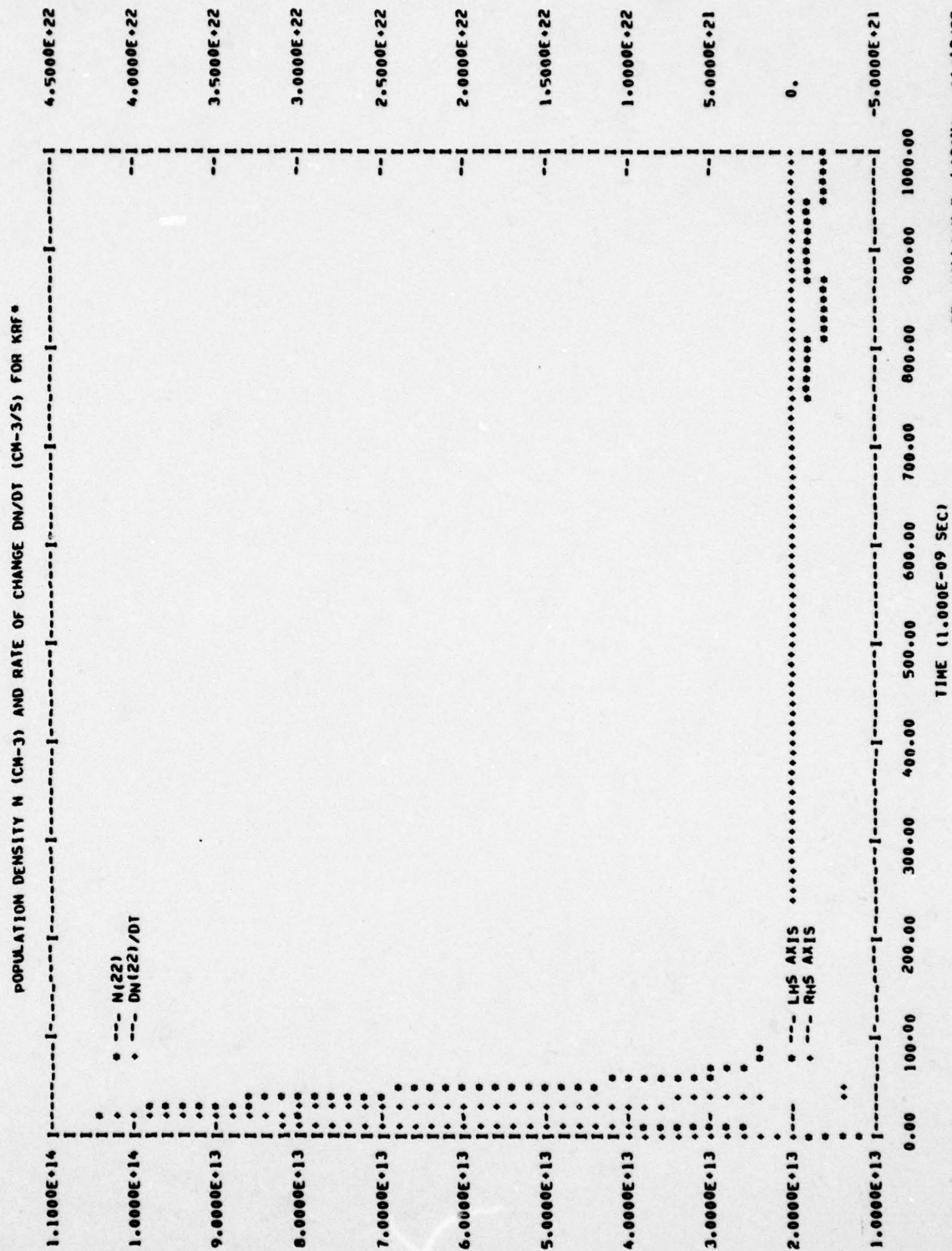


Fig. 4.35: Population density and rate of change for KrF\*.

DR. WILLIAM B. LACINA, 01/12/79  
 NORTHROP RESEARCH AND TECHNOLOGY

### 4.3 Error Diagnostic Assistance

Although it is not possible to anticipate all possible forms of incorrect usage, program LASER has been designed to provide limited diagnostic assistance upon recognition of certain (potential) error conditions. The search for errors occurs in processing an input reaction queue for subroutine synthesis, and at the time of data input for execution of the analysis.

The DATA BLOCK 1 shown in Fig. 4.36 violates several of the conventions described in Sec. 3.2. Assume that program LASER has been dimensioned  $NMAX = 30$ ,  $KMAX = 16$ , and  $NKMAX = 8$  (for purposes of illustration), and that DATA BLOCK 1 is submitted for a program synthesis. Even if the reaction syntax contained no intrinsic defects, its species content and total length would exceed the dimension capacity specified for LASER.

The reaction summary generated in an attempt to process the DATA BLOCK 1 of Fig. 4.36 contains numerous informative and diagnostic comments, as shown in Fig. 4.37. For defective reactions, there is no FORTRAN translation; the reaction is ignored (and unnumbered in Fig. 4.37), and processing continues. The data file generated (unit 4) contains, in addition to the rate constant data, a logical parameter (written in the second record) whose value is `.TRUE.` or `.FALSE.` depending upon whether or not errors were encountered. A later attempt to execute an incomplete analysis from which reactions were rejected can be prohibited by specifying `FATAL(1) = .TRUE.`

Return now to the KrF program, synthesized from the reaction scheme of Fig. 4.1 to produce the subroutines illustrated in Fig. 4.2 - 4.4. For



the purpose of illustrating execution error diagnostics, suppose that the original kinetic scheme of Fig. 4.1 had contained some (unimportant) error, such as the rejection of a duplicate reaction. (Thus, for all practical purposes, files KRFB CD and KRFLASER are completely satisfactory, although KRFDATA will contain a record of the fact that a defect had been encountered during synthesis.) Suppose, furthermore, that the dimension declarators in LASER have been changed since the original creation of the KrF files, and that execution of the analysis is attempted with the input DATA BLOCK 4 shown in Fig. 4.38. Note that no specification of the vector FATAL(I) appears in the data group \$CONTROL ... \$ to override the default initialization .FALSE. Note further that Fig. 4.38 differs from Fig. 4.7 in that now, there are rate constant modifications specified by \$RATES ... \$ entry, and a new species "XXX" has been initialized. (Most of the other parameters are numerically different, but that is not relevant for the point to be illustrated here.) Fig. 4.39 is the tabular summary of the reaction scheme and its modified rate constants; note that some of the attempted modifications were illegal and were rejected. Fig. 4.40 is a summary of error diagnostics encountered in the attempt to execute the analysis.

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK  
(DATE: 02/02/79)

CARD NO.	1	2	3	4	5	6	7	8
	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

1 ....TEST CASE CONTAINING ERRORS  
2 ....AR2F\* + F2 \* AR + KR + F + F2  
3 ....1.00 E-09 SRI REPORT, DEC. 1976.  
4 ....F2 + AR2F\* + F\*F2 + KR + AR  
5 ....1.00 E-09 SRI REPORT, DEC. 1976.  
6 ....XY + E \* XY\*\* + E  
7 ....  
8 ....XY + E \* XY\* + E  
9 ....1.00 E-08 1.40 E-09  
10 ....AR + E \* AR\* + E  
11 ....  
12 ....AR + E \* AR(+) + E + E  
13 ....  
14 ....KR + E \* KR\* + E  
15 ....  
16 ....KR + E \* KR(+) + E + E  
17 ....  
18 ....XY + E \* XY(+) + E  
19 ....  
20 ....XY + E \* XY\* + E  
21 ....1. 1.  
22 ....AR\* + E \* AR(+) + E + E  
23 ....  
24 ....KR\* + E \* KR(+) + E + E  
25 ....  
26 ....AR\*\* +E- \* AR(+) + 2E-  
27 ....  
28 ....KR\*\* + E- \* KR(+) + E- + E-  
29 ....  
30 ....XY + E \* XY\* + E + E  
31 ....  
32 ....XY\* + E \* XY + E  
33 ....1. 1.  
34 ....KR2(+) + E \* KR + KR\*  
35 ....  
36 ....AR2(+) + E \* AR + AR\*  
37 ....  
38 ....F2 + E \* F + F-  
39 ....  
40 ....AR(+) + E \* AR(2+) + E + E

AN ANONYMOUS SOURCE  
REFERENCE: PHYS. REV. 12, 22 (1728)  
RAPP, ENGLANDER-GOLDEN, J. CHEM PHYS. 43,1464 (65)  
SCHAPER, SCHEIBNER, BEITR. AUS PLASMA PHYS. 9, 45  
DECREED BY VOTE OF THE LEGISLATURE  
FROM A USUALLY UNRELIABLE SOURCE

1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
1	2	3	4	5	6	7	8

Fig. 4.36: Defective DATA BLOCK 1.

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK  
(DATE: 02/02/79)

CARD NO.	1	2	3	4	5	6	7	8
	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

```

41 ... 1. 1.
42 ...AR(+) * E * AR(++) * E * E
43 ... 1. 1.
44 ...AR * KR * KR * AR*
45 ... 1.
46 ...A * B * XYZ --> AX * BY * Z
47 ... 4.50 E-10 5.00 E-09 KNOWN SINCE ANTIQUITY
48 ...AR(+) * KR * AR * KR(+)
49 ... 3.00 E-11
50 ...KR2* * M * KR * KR
51 ... 1.
52 ...KR2* * M * KR * KR * M
53 ... 1. 1.
54 ...XY * ME- * XY(+) * ME- * ME-
55 ... 1. 1.
56 ...AR * ME- * AR(+) * ME- * E-
57 ... 1. 1.
58 ...A * XY * B * C * AR * KR * A* * XY(+) * E * B * C * AR * KR*
59 ... 1. 1.
60 ...KR* * AR * AR* * KR
61 ... 1. 2.
62 ...KRF* * RAD * KR * F * RAD
63 ... 1. 1. STIMULATED EMISSION PROCESS.
64 ...XY* * X * Y* * RAD
65 ... 1. 1.
66 ...F- * RAD * F * E
67 ... 5.40 E-10 A. HANDL. PHYS. REV. A3. 251 (1971)
68 ...KRF* * KR * F * WNU BURNHAM AND SEARLES
69 ... 1.10 E 00
70 ...XY* * XY
71 ... 1. 1.
72 ... AB * E * A * B * E
73 ... 1. 1.

```

1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
1	2	3	4	5	6	7	8

Fig. 4.36: Defective DATA BLOCK 1 (cont'd).



# SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1), CH3/SEC, CH6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS		RATE REFERENCES AND/OR COMMENTS
		KF(I)	KR(I)	
1	AR2F + F2 + AR + KR + F + F2	1.0000E-09		SRI REPORT, DEC. 1976. REVERSE REACTION IS IGNORED -- KR = 0.
	F2 + AR2F + F + F2 + KR + AR	1.0000E-09		SRI REPORT, DEC. 1976. REACTION IGNORED -- SAME AS NUMBER 1. REVERSE REACTION IS IGNORED -- KR = 0.
2	XY + E + XY00 + E	(COMPUTED)	(COMPUTED)	AN ANONYMOUS SOURCE WARNING -- NO E- CROSS SECTION DATA WAS FOUND. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
3	XY + E + XY0 + E	1.0000E-08	1.4000E-09	REFERENCE: PHYS. REV. 12, 22 (1978)
4	AR + E + AR0 + E	(COMPUTED)	(COMPUTED)	FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
5	AR + E + AR(+) + E + E	(COMPUTED)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J. CHEM PHYS 43 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
6	KR + E + KR0 + E	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
7	KR + E + KR(+) + E + E	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
	XY + E + XY(+) + E			DECREED BY VOTE OF THE LEGISLATURE REACTION REJECTED -- CHARGE CONSERVATION VIOLATED.
	XY + E + XY0 + E	1.0000E+00	1.0000E+00	FROM A USUALLY UNRELIABLE SOURCE REACTION IGNORED -- SAME AS NUMBER 3.
8	AR0 + E + AR(+) + E + E	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
9	KR0 + E + KR(+) + E + E	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 02/02/79

Fig. 4.37: Summary of defective reaction scheme.

# SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CH3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I) KR(I)	RATE REFERENCES AND/OR COMMENTS
	AR <sup>00</sup> + E <sup>-</sup> → AR(I <sup>0</sup> ) + 2E <sup>-</sup>		REACTION REJECTED -- CHARGE CONSERVATION VIOLATED. REVERSE REACTION IS IGNORED -- KR = 0.
10	KR <sup>00</sup> + E <sup>-</sup> → KR(I <sup>0</sup> ) + E <sup>-</sup> + E <sup>-</sup>	(COMPUTED)	FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
	XY + E <sup>-</sup> → XY <sup>0</sup>		BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED.
	XY <sup>0</sup> + E <sup>-</sup> → XY + E <sup>-</sup>	1.0000E+00	REACTION IGNORED -- REVERSE OF NO. 3.
	KR2(I <sup>0</sup> ) + E <sup>-</sup> → KR + KR <sup>0</sup>		REACTION REJECTED -- NO MORE THAN 8 REACTIONS ARE ALLOWED FOR THE COUPLED E- KINETICS ANALYSIS. REVERSE REACTION IS IGNORED -- KR = 0.
	AR2(I <sup>0</sup> ) + E <sup>-</sup> → AR + AR <sup>0</sup>		REACTION REJECTED -- NO MORE THAN 8 REACTIONS ARE ALLOWED FOR THE COUPLED E- KINETICS ANALYSIS. REVERSE REACTION IS IGNORED -- KR = 0.
	F2 + E <sup>-</sup> → F + F <sup>-</sup>		REACTION REJECTED -- NO MORE THAN 8 REACTIONS ARE ALLOWED FOR THE COUPLED E- KINETICS ANALYSIS. REVERSE REACTION IS IGNORED -- KR = 0.
	AR(I <sup>0</sup> ) + E <sup>-</sup> → AR(2 <sup>0</sup> ) + E <sup>-</sup> + E <sup>-</sup>	1.0000E+00	REACTION REJECTED -- CHARGE CONSERVATION VIOLATED. E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
11	AR(I <sup>0</sup> ) + E <sup>-</sup> → AR(I <sup>00</sup> ) + E <sup>-</sup> + E <sup>-</sup>	1.0000E+00	E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
12	AR + KR <sup>0</sup> → KR + AR <sup>0</sup>	1.0000E+00	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	A + B + XYZ → AX + BY + Z		KNOWN SINCE ANTIQUITY BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED.
13	AR(I <sup>0</sup> ) + KR → AR + KR(I <sup>0</sup> )	3.0000E-11	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	KR2 <sup>0</sup> + M → KR + KR	1.0000E+00	IMPROPER BUFFER GAS SPECIFICATION. BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED. REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
14	KR2 <sup>0</sup> + M → KR + KR + M	1.0000E+00	

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY, DATE: 02/02/79

Fig. 4.37: Summary of defective reaction scheme (cont'd).



# SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, .... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS		RATE REFERENCES AND/OR COMMENTS
		KF(I)	KR(I)	
		(IGNORED REACTIONS ARE NOT NUMBERED)		
	XY + HE- -> XY(I) + HE- + HE-	1.0000E+00	1.0000E+00	IMPROPER HIGH ENERGY ELECTRON TERMS. BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED. REACTION REJECTED -- CHARGE CONSERVATION VIOLATED.
15	AR + HE- -> AR(I) + HE- + E- A + XY + B + C + AR + KR	1.0000E+00	1.0000E+00	E- CREATION ASSUMED TO BE OVER ENERGY DISTRIBUTION > 5 SPECIES ON LHS OR RHS NOT PERMITTED. BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED.
16	KR + AR -> AR + KR KRF + RAD -> KR + F + RAD XY + X + Y + RAD F- + RAD -> F + E	1.0000E+00 1.0000E+00 1.0000E+00 5.4000E-10	2.0000E+00 1.0000E+00 1.0000E+00	REACTION IGNORED -- SAME AS NUMBER 12. STIMULATED EMISSION PROCESS. THIS RADIATIVE PROCESS NOT ALLOWED. MORE THAN 16 REACTIONS ARE IGNORED. A. MANDEL. PHYS. REV. A3, 251 (1971) MORE THAN 16 REACTIONS ARE IGNORED. E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
	KRF + KR + F + HNU	1.1000E+00		BURNHAM AND SEARLES MORE THAN 16 REACTIONS ARE IGNORED. REVERSE REACTION IS IGNORED -- KR = 0. NO REVERSE REACTION ALLOWED FOR RADIATIVE DECAY. MORE THAN 16 REACTIONS ARE IGNORED.
	XY + XY	1.0000E+00	1.0000E+00	MORE THAN 16 REACTIONS ARE IGNORED.
	AB + E + A + B + E	1.0000E+00	1.0000E+00	REACTION IS IGNORED -- MORE THAN 20 DIFFERENT GAS SPECIES ARE NOT PERMITTED WITH PRESENT DIMENSION. MORE THAN 16 REACTIONS ARE IGNORED.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHRUP RESEARCH AND TECHNOLOGY. DATE: 02/02/79

OF 36 INPUT REACTIONS SCANNED, 16 WERE RETAINED (MAXIMUM ALLOWED = 16) AND 20 WERE IGNORED FOR REASONS ITEMIZED IN THE TABLE.  
OF THOSE RETAINED, 8 REQUIRE RATES FROM AN E- KINETICS ANALYSIS. 18 SEPARATE SPECIES WERE ENCOUNTERED (MAXIMUM ALLOWED = 20).  
ERRORS WHICH WERE DETECTED IN PROCESSING THE INPUT REACTION SCHEME MAY CAUSE PROGRAM TERMINATION IF THEY HAVE BEEN SPECIFIED TO  
BE TREATED AS FATAL. MODIFICATIONS OF THE REACTION SCHEME, CORRECTIONS IN REACTION SYNTAX, CHANGES IN DIMENSION STORAGE, OR  
ADDITIONS TO THE E- CROSS SECTION FILE MAY BE REQUIRED TO REMOVE ALL OF THE ERROR DECLARATIONS.

Fig. 4.37: Summary of defective reaction scheme (cont'd).



CARD NO. 1 2 3 4 5 6 7

1	....					IO(1) = 1,1,1,1,1,1,10,0,0,1,	
2	....					EMAX = 20.,	
3	....					NMCYCLE = 200.	
4	....					LIMIT = 5\$	
5	....					TPULSE = 1.0E-06,	
6	....					ATM = 1.7\$	
7	....	SOPTICAL				REFLECT = 70.,	
8	....					LOSS = 0.,	
9	....					AREA = 25.,	
10	....					CAVITY = 130.,	
11	....	SEBEAM				LENGTH = 75.0\$,	
12	....					JBEAM = 12.0.,	
13	....					ENERGY = 320.,	
14	....					UB = 20.,	
15	....					TB(1) = 0., .50., .100., .150., .200., .250., .300.,	
16	....					.350., .40., .450., .500., .550., .600., .650.,	
17	....					.700., .750., .800., .850., .900., .950., .1000.,	
18	....					UNITS = 1.0F-09,	
19	....					JB(1) = 0., .62, 1., .1., .9., .85., .77., .73., .69.,	
20	....					.67., .69., .72., .75., .75., .72., .65., .42., .2.,	
21	....					.05., .02, 0.,	
22	....					FACTOR = 2.0\$,	
23	....	SCIRCUIT				CAPAC = 1.33E-06,	
24	....					INDUCT = 200.E-09,	
25	....					RESIST = 0.,	
26	....					KVOLT = 40.,	
27	....					AREA = 2000.,	
28	....					DIST = 10.\$	
29	....					KF(9) = 1.,	
30	....					KR(12) = 1.,	
31	....					KF(17) = 1.E-07,	
32	....					KR(26) = 1.,	
33	....					KF(44) = 6.2E-12,6.0E-32,	
34	....					KR(50) = 0.\$	
35	....	..AR				1191.	40.
36	....	..KR				100.	84.
37	....	..F2				1.5	38.
38	....	..AR*				11.5	PLOT
39	....	..KR*				9.9	
40	....	..AR2(*)				13.0	

[illegible]

**CONTINUED**

**Fig. 4.38: DATA BLOCK 4 input for illustration of error diagnostics.**

CARD NO. 1 2 3 4 5 6 7 A  
12345678901234567890123456789012345678901234567890

[illegible]

**Fig. 4.38 (Continued)**

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSI(K,1) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
1	AR + E → AR* + E	VSI(1, 1)	VSI(2, 1)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
2	KR + E → KR* + E	VSI(1, 2)	VSI(2, 2)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
3	AR + E → AR** + E	VSI(1, 3)	VSI(2, 3)	0.1 X CROSS SECTION FOR AR + E → AR* + F IS ASSUME
4	KR + E → KR** + E	VSI(1, 4)	VSI(2, 4)	0.1 X CROSS SECTION FOR KR + E → KR* + F IS ASSUME
5	AR* + E → AR** + E	VSI(1, 5)	VSI(2, 5)	VRIENS CROSS SECTION
6	KR* + E → KR** + E	VSI(1, 6)	VSI(2, 6)	VRIENS CROSS SECTION
7	AR + E → AR(+) + E + E	VSI(1, 7)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43
8	KR + E → KR(+) + E + E	VSI(1, 8)		KIEFFER REPORT, P. 16
9	AR* + E → AR(+) + E + E	VSI(1, 9)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
10	KR* + E → KR(+) + E + E	VSI(1, 10)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
11	AR** + E → AR(+) + E + E	VSI(1, 11)		VRIENS CROSS SECTION
12	KR** + E → KR(+) + E + E	VSI(1, 12)		VRIENS CROSS SECTION
13	AR2(+) + E → AR* + AR	VSI(1, 13)		MEHR AND BIONDI: SYNTHETIC CROSS SECTION FOR TE**
14	KR2(+) + E → KR* + KR	VSI(1, 14)		OSKAM, MITTELSTADT: SYNTHETIC, TE**(-2/3) LAW.
15	F2 + E → F + F-	VSI(1, 15)		AEROSPACE (PRIVATE COMMUN.)
16	AR2* + E → AR + AR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
17	KR2* + E → KR + KR + E	1.0000E-07		**** THE ORIGINAL RATE HAS BEEN MODIFIED *****
18	AR + HE- → AR(+) + HE- + E	4.3400E-18		BERGER-SELTZER: STOP = 1.7 MEVCM2/GM (300 KEV)
19	AR + HE- → AR* + HE-	1.2400E-18	1.2400E-18	(1/3.5) X AR + HE → AR(+) + E + HE
20	KR + HE- → KR(+) + HE- + E	8.0400E-18		BERGER-SELTZER: STOP = 1.5 MEVCM2/GM (300 KEV)

\* THE ORIGINAL RATE CONSTANT(S) HAVE BEEN MODIFIED  
\*\* ILLEGAL ATTEMPT TO MODIFY RATE CONSTANT(S) WAS REJECTED

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme.



SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
21	KR * HE- * KR * HE-	2.3000E-10	2.3000E-10	(1/3.5) * KR * HE * KR(1) * E * HE
22	AR(1) * AR * M * AR2(1) * M	2.0000E-31		W. F. LIU, D. C. CONWAY JCP 62, 3070 (1975)
23	AR(1) * KR * M * ARKR(1) * M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
24	KR(1) * KR * M * KR2(1) * M	2.4000E-31		C. J. TRACY, M. J. OSKAM JCP 65, 3387 (1976)
25	KR(1) * AR * M * ARKR(1) * M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
26	AR(1) * KR * AR * KR(1)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
27	AR2(1) * KR * KR(1) * AR * AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
28	ARKR(1) * KR * KR2(1) * AR	3.2000E-10	X E(-E/KT)	BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
29	AR * AR * M * AR2 * M	1.0000E-32		HILL, GUTCHECK, HUESTIS, ET AL. SRI REPORT, 1974.
30	AR * KR * M * ARKR * M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
31	KR * KR * M * KR2 * M	5.5000E-32		HUGHES LASL ASPEN 9/76
32	KR * AR * M * ARKR * M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
33	ARKR * KR * KR2 * AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 7A-99, DEC., 1976
34	AR2(1) * F- * ARF * AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
35	AR2(1) * F- * AR2F *	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
36	AR(1) * F- * ARF *	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
37	KR2(1) * F- * KRF * KR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
38	KR2(1) * F- * KR2F *	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
39	KR(1) * F- * KRF *	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
40	ARKR(1) * F- * KRF * AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

\*\* ILLEGAL ATTEMPT TO MODIFY RATE CONSTANT(S) WAS REJECTED

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme.  
(Continued)

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K=1) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
41	ARKR(1) * F * ARKRF	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
42	KR * F2 * KRF * F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
43	AR * F2 * ARF * F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
44	AR * KR * AR * KR	6.2000E-12	X E(-E/KT)	***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
45	KRF * AR * M * ARKRF * M	6.0000E-32		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
46	KRF * KR * M * KR2F * M	5.0000E-31		AVCO
47	ARF * AR * M * AR2F * M	4.0000E-31		AVCO
48	ARF * KR * M * ARKRF * M	1.0000E-31		
49	AR2 * KR * AR * AR * KR	9.0000E-11		REVERSE REACTION IS IGNORED -- KR = 0.
50	AR2 * AR2 * AR2(1) * AR * AR * E	3.0000E-10		ZAMIN (PRIV. COMMUN. TO SRI)
51	ARF * KR * KRF * AR	1.5000E-10	X E(-E/KT)	E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
52	AR2 * F * ARF * AR	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
53	KR2 * F * KRF * KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
54	AR2 * F2 * AR2F * F	2.5000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
55	ARKR * F2 * KRF * AR * F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976
56	ARKR * F2 * ARKRF * F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
57	KR2 * F2 * KR2F * F	3.0000E-10	X E(-E/KT)	
58	AR2F * F2 * AR * AR * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
59	ARKRF * F2 * AR * KR * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
60	KR2F * F2 * KR * KR * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976

\* THE ORIGINAL RATE CONSTANT(S) HAVE BEEN MODIFIED  
\*\* ILLEGAL ATTEMPT TO MODIFY RATE CONSTANT(S) WAS REJECTED

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme.  
(Continued)



SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79  
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA  
(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
61	ARKRF • KR • KR2F • AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
62	KRF • F2 • KR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
63	ARF • F2 • AR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
64	AR2F • KR • KRF • AR • AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
65	AR • M • AR • M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
66	KR • M • KR • M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
67	ARF • AR • F	3.3000E-07		SRI REPORT NO. MP 76-99, DEC., 1976
68	AR2 • AR • AR	3.8000E-06		SRI REPORT NO. MP 76-99, DEC., 1976
69	ARKR • AR • KR	3.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
70	KR2 • KR • KR	3.3000E-06		SRI REPORT NO. MP 76-99, DEC., 1976
71	AR2F • AR • AR • F	2.0000E-08		SRI REPORT NO. MP 76-99, DEC., 1976
72	ARKRF • AR • KR • F	5.0000E-07		SRI REPORT NO. MP 76-99, DEC., 1976
73	KR2F • KR • KR • F	6.7000E-07		SRI REPORT NO. MP 76-99, DEC., 1976
74	KRF • KR • F • HNU	1.1000E-08		R. BURNHAM, S. S. SEARLES (SUBMITTED TO JCP)
75	KRF • RAD • KR • F • RAD	2.0000E-16		LASER TRANSITION; STIMULATED EMISSION X-SECTION
76	F2 • RAD • F • F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
77	F • RAD • F • E	5.4000E-18		A. MANOL, PHYS REV A3, 251 (1971)
78	KR2F • RAD • AR • KR • F	1.0000E-99		CROSS SECTION UNKNOWN
79	AR2(•) • RAD • AR • AR(•)	1.5000E-17		STEVENS (PARK CITY CONFERENCE)
80	KR2(•) • RAD • KR • KR(•)	3.5000E-18		J. WEST (NRTC)

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme.  
(Continued)



# SUMMARY OF POSSIBLE ERROR CONDITIONS

SEVERITY

DESCRIPTION

WARNING:

ERRORS WERE DETECTED IN PROCESSING THE INPUT REACTION SCHEME. MODIFICATIONS OF THE REACTION SCHEME, CORRECTIONS IN REACTION SYNTAX, CHANGES IN DIMENSION STORAGE, OR ADDITIONS TO THE E-CROSS SECTION FILE MAY BE REQUIRED TO REMOVE ALL OF THE ERROR CONDITIONS.

WARNING:

SYNTHESIZED SUBROUTINES AND DATA FILE WERE GENERATED WITH DIMENSION DECLARATIONS MMAX = 30, KMAX = 200, AND NKMAX = 25. THESE MUST AGREE WITH THE CORRESPONDING DIMENSION DECLARATIONS IN THE MAIN PROGRAM (LASER). EXECUTION MAY BE POSSIBLE IF PRESENT STORAGE EXCEEDS ORIGINAL, BUT CAUTION IS ADVISED TO INSURE THAT LABELED COMMON BLOCKS AGREE WITH THOSE IN THE SYNTHETIC SUBROUTINES ASSOCIATED WITH THE DATA FILE GENERATED ON TAPE4.

WARNING:

TAPE4 DATA FILE VECTORS EXCEEDED DIMENSION STORAGE IN MAIN PROGRAM, AND WERE TRUNCATED DURING READ. MMAX = 25, KMAX = 200, AND NKMAX = 30. TAPE4 CONTAINS NK = 15, KTYPE = 80, AND NTYPE = 24. CAUTION IS ADVISED.

WARNING:

AN ATTEMPT WAS MADE TO ENTER, BY SRATES ... \$ INPUT, THE FOLLOWING RATES, WHICH ARE NOT ACCESSIBLE BY INPUT FOR THE SYNTHETIC PROGRAM THAT WAS GENERATED. IF THE PROGRAM EXECUTES, THE ATTEMPTED MODIFICATIONS WILL BE IGNORED, AND THE ORIGINAL RATES USED:

KF( 9) KR( 12) KR( 26) KR( 50)

WARNING:

THE FOLLOWING SPECIES WERE INITIALIZED BY INPUT DATA, BUT DID NOT OCCUR IN THE KINETIC SYSTEM. IF THE PROGRAM IS EXECUTED, THEY WILL BE IGNORED, BUT INCLUDED IN THE TOTAL PRESSURE (AS BUFFER GASES IN 3-BODY COLLISIONS) AND FOR MOMENTUM TRANSFER IN E-KINETICS ANALYSIS:

xxx

WARNING:

INITIAL POPULATION DENSITIES FOR THE FOLLOWING SPECIES WERE NOT DEFINED. IF THE PROGRAM IS EXECUTED, NO(1) = 0 WILL BE ASSUMED:

RAD	AR*	KR*	AR**	KR**	AR(1)	KR(1)	AR2(1)
KR2(1)	F	F-	AR2*	KR2*	ARKR(1)	ARKR*	ARF*
AR2F*	KRF*	KR2F*	ARKRF*				

WARNING:

ENERGIES FOR THE FOLLOWING SPECIES WERE NOT DEFINED. IF PROGRAM IS EXECUTED, E(1) = 0 WILL BE ASSUMED:

AR	KR	F2	F
----	----	----	---

Fig. 4.40: Execution error diagnostics illustrated.

# SUMMARY OF POSSIBLE ERROR CONDITIONS

SEVERITY	DESCRIPTION
WARNING:	<p>ERRORS OCCURRED FOR THE INPUT CROSS SECTIONS FOR THE FOLLOWING ELECTRON COLLISION PROCESSES.  IF THE PROGRAM IS EXECUTED, A ZERO CROSS SECTION OVER ALL ENERGY WILL BE ASSUMED</p> <p>1) MOMENTUM TRANSFER FOR F2  NO E- CROSS SECTION DATA WAS FOUND.</p> <p>2) MOMENTUM TRANSFER FOR XXX  NO E- CROSS SECTION DATA WAS FOUND.  THE MASS ENTERED FOR THIS SPECIES IS 1 0</p>
FATAL:	<p>MOMENTUM TRANSFER COLLISION FREQUENCY IS ZERO AT SOME POINT. E- ANALYSIS CONTAINS 1/0N TERMS.</p> <p>PROGRAM IS TERMINATED FOR ERRORS SPECIFIED FATAL.</p>

Fig. 4.40: Execution error diagnostics (continued)

## 5.0 REFERENCES

1. W. B. Lacina and R. S. Bradford, Jr., "Kinetic Modeling of Electrical Lasers: Results for KrF", presented at Twenty Ninth Gaseous Electronics Conference, Cleveland, Ohio, October, 1976.
2. W. B. Lacina, D. B. Cohn, R. S. Bradford, Jr., J. B. West, D. Richman, W. H. Long, and M. L. Bhaumik, "High Power Rare Gas Halide Laser Investigations", presented at Seventh Winter Colloquium on High Power Visible Lasers, Park City, Utah, February, 1977.
3. W. B. Lacina, R. S. Bradford, Jr., and M. L. Bhaumik, Kinetic Studies of the KrF Laser, Northrop Rept. # NRTC-77-29R, March, 1977.
4. W. B. Lacina and D. B. Cohn, "Theoretical Analysis of the Electrically Excited KrF Laser," Appl. Phys. Lett. 32, 106 (1978).
5. D. B. Cohn and W. B. Lacina, High Power Short Wavelength Laser Development, Northrop Rept. # NRTC-77-43R, November, 1977.
6. C. W. Gear, Numerical Initial Value Problems in Ordinary Differential Equations, Prentice Hall, Englewood Cliffs, N. J. (1971), pp. 155-167.
7. T. Holstein, "Energy Distribution of Electrons in High Frequency Gas Discharges," Phys. Rev. 70, 367 (1946).
8. W. P. Allis, "Motions of Ions and Electrons," in Handbuch der Physik, Vol. XXI, Springer-Verlag, Berlin (1956).
9. I. P. Schkarofsky, T. W. Johnston, and M. P. Bachynski, The Particle Kinetics of Plasmas, Addison-Wesley, Mass. (1966).
10. L. S. Frost and A. V. Phelps, "Rotational Excitation and Momentum Transfer Cross Sections for Electrons in  $H_2$  and  $N_2$  from Transport Coefficients," Phys. Rev. 127, 1621 (1962).
11. N. P. Carleton and L. R. Megill, "Electron Energy Distributions in Slightly Ionized Air under the Influence of Electric and Magnetic Fields," Phys. Rev. 126, 2089 (1962).



12. A. G. Englehardt and A. V. Phelps, "Elastic and Inelastic Collision Cross Sections in Hydrogen and Deuterium from Transport Coefficients," *Phys. Rev.* 131, 2115 (1963).
13. A. G. Englehardt, A. V. Phelps, and C. G. Risk, "Determination of Momentum Transfer and Inelastic Cross Sections for Electrons in Nitrogen using Transport Coefficients," *Phys. Rev.* A135, 1566 (1964).
14. W. L. Nighan, "Electron Energy Distributions and Collision Rates in Electrically Excited  $N_2$ , CO, and  $CO_2$ ," *Phys. Rev.* 2A, 1989 (1970); "Electron Kinetic Processes in CO Lasers," *Appl. Phys. Lett.* 20, 96 (1972); W. L. Nighan and J. H. Bennett, "Electron Energy Distribution Functions and Vibrational Excitation Rates in  $CO_2$  Laser Mixtures," *Appl. Phys. Lett.* 14, 240 (1969).
15. S. D. Rockwood, "Elastic and Inelastic Cross Sections for Electron-Hg Scattering from Hg Transport Data," *Phys. Rev.* A8, 2348 (1973).
16. J. H. Hancock, R. C. Jones, and C. B. Mills, "Numerical Solution of the Boltzmann Equation for Energy Distributions of Electrons with Inelastic Scattering on Molecules," Los Alamos Rept. # LA-4832, May, 1972.
17. C. J. Elliott, O. P. Judd, A. M. Lockett, and S. D. Rockwood, "Electron Transport Coefficients and Vibrational Excitation Rates for Electrically Excited  $CO_2$  Gas Lasers," Los Alamos Informal Rept. # LA-5562-MS, April, 1974.
18. W. L. Morgan and E. L. Fisher, "Calculations on the Electron Energy Distribution in a Molecular Laser Plasma, Research Institute for Engineering Sciences, Wayne State University, Rept. # RIES 74-56, August, 1974.
19. J. J. Lowke, A. V. Phelps, and B. W. Irwin, "Predicted Electron Transport Coefficients and Operating Characteristics of  $CO_2$ - $N_2$ -He Laser Mixtures," *J. Appl. Phys.* 44, 4664 (1973).
20. W. B. Lacina, "Supersonic Continuous Wave Carbon Monoxide Laser Development, Phase I. Volume I: CO Laser Kinetics Code, and Volume IV: Rates and Cross Sections," Northrop Rept. No. NRTC-75-25R, July, 1975.

21. W. F. Bailey, "Electron Kinetic Processes in N<sub>2</sub> Discharges," presented at Twenty-Fifth Gaseous Electronics Conf., London, Ontario, Canada, October, 1972 (Paper DD5).
22. W. H. Long, "Electron Kinetics in the KrF Laser," Appl. Phys. Lett. 31, 391 (1977).
23. M. J. Berger and S. M. Seltzer, Studies in Penetration of Charged Particles in Matter, National Acad. Sci. Publ. No. 1133, Chapt. 10 (1967).